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A UNITED STATES  
DEPARTMENT OF  
COMMERCE  
PUBLICATION



# NBS SPECIAL PUBLICATION 305

## SUPPLEMENT 4

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# PUBLICATIONS

## OF THE NATIONAL BUREAU OF STANDARDS

U.S.  
DEPARTMENT  
OF  
COMMERCE

National  
Bureau  
of  
Standards

# 1972 CATALOG

## NATIONAL BUREAU OF STANDARDS

The National Bureau of Standards<sup>1</sup> was established by an act of Congress March 3, 1901. The Bureau's overall goal is to strengthen and advance the Nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research and provides: (1) a basis for the Nation's physical measurement system, (2) scientific and technological services for industry and government, (3) a technical basis for equity in trade, and (4) technical services to promote public safety. The Bureau consists of the Institute for Basic Standards, the Institute for Materials Research, the Institute for Applied Technology, the Institute for Computer Sciences and Technology, and the Office for Information Programs.

**THE INSTITUTE FOR BASIC STANDARDS** provides the central basis within the United States of a complete and consistent system of physical measurement; coordinates that system with measurement systems of other nations; and furnishes essential services leading to accurate and uniform physical measurements throughout the Nation's scientific community, industry, and commerce. The Institute consists of a Center for Radiation Research, an Office of Measurement Services and the following divisions:

Applied Mathematics — Electricity — Mechanics — Heat — Optical Physics — Nuclear Sciences<sup>2</sup> — Applied Radiation<sup>2</sup> — Quantum Electronics<sup>3</sup> — Electromagnetics<sup>3</sup> — Time and Frequency<sup>3</sup> — Laboratory Astrophysics<sup>3</sup> — Cryogenics<sup>3</sup>.

**THE INSTITUTE FOR MATERIALS RESEARCH** conducts materials research leading to improved methods of measurement, standards, and data on the properties of well-characterized materials needed by industry, commerce, educational institutions, and Government; provides advisory and research services to other Government agencies; and develops, produces, and distributes standard reference materials. The Institute consists of the Office of Standard Reference Materials and the following divisions:

Analytical Chemistry — Polymers — Metallurgy — Inorganic Materials — Reactor Radiation — Physical Chemistry.

**THE INSTITUTE FOR APPLIED TECHNOLOGY** provides technical services to promote the use of available technology and to facilitate technological innovation in industry and Government; cooperates with public and private organizations leading to the development of technological standards (including mandatory safety standards), codes and methods of test; and provides technical advice and services to Government agencies upon request. The Institute consists of a Center for Building Technology and the following divisions and offices:

Engineering and Product Standards — Weights and Measures — Invention and Innovation — Product Evaluation Technology — Electronic Technology — Technical Analysis — Measurement Engineering — Structures, Materials, and Life Safety<sup>4</sup> — Building Environment<sup>4</sup> — Technical Evaluation and Application<sup>4</sup> — Fire Technology.

**THE INSTITUTE FOR COMPUTER SCIENCES AND TECHNOLOGY** conducts research and provides technical services designed to aid Government agencies in improving cost effectiveness in the conduct of their programs through the selection, acquisition, and effective utilization of automatic data processing equipment; and serves as the principal focus within the executive branch for the development of Federal standards for automatic data processing equipment, techniques, and computer languages. The Center consists of the following offices and divisions:

Information Processing Standards — Computer Information — Computer Services — Systems Development — Information Processing Technology.

**THE OFFICE FOR INFORMATION PROGRAMS** promotes optimum dissemination and accessibility of scientific information generated within NBS and other agencies of the Federal Government; promotes the development of the National Standard Reference Data System and a system of information analysis centers dealing with the broader aspects of the National Measurement System; provides appropriate services to ensure that the NBS staff has optimum accessibility to the scientific information of the world. The Office consists of the following organizational units:

Office of Standard Reference Data — Office of Technical Information and Publications — Library — Office of International Relations.

<sup>1</sup> Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.

<sup>2</sup> Part of the Center for Radiation Research.

<sup>3</sup> Located at Boulder, Colorado 80302.

<sup>4</sup> Part of the Center for Building Technology.



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# Publications of the National Bureau of Standards 1972 Catalog

## A Compilation of Abstracts and Key Word and Author Indexes

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Betty L. Oberholtzer

Office of Technical Publications  
National Bureau of Standards  
Washington, D.C. 20234

<sup>t</sup> Special publication no. 350, Supplement 4



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U.S. DEPARTMENT OF COMMERCE, Frederick B. Dent, *Secretary*

U.S. NATIONAL BUREAU OF STANDARDS, Richard W. Roberts, *Director*

Issued July 1973

## National Bureau of Standards Special Publication 305 Supplement 4

To Accompany National Bureau of Standards Circular 460; its Supplement, Miscellaneous Publication 240; its Supplement, Special Publication 305; and its Supplements 1, 2, and 3

Nat. Bur. Stand. (U.S.), Spec. Publ. 305 Suppl. 4, 449 pages (July 1972)

CODEN: XNBSAV



## PREFACE

All National Bureau of Standards papers published in NBS and non-NBS media during 1972 are cited in this annual supplement to the NBS publications catalog. About one-fourth of these papers were issued in the Bureau's own publications series; the remaining three-fourths were published in non-NBS media: various professional and technical journals and books. From the viewpoint of published pages rather than papers, about three-fourths of the total appeared in the Bureau's own publications series.

As in past supplements, the citations for all NBS papers, whatever the publication medium, include full title, author(s), place of publication, abstract, and key words. Permuted author and key word indexes are included to facilitate use of the catalog and to enhance its value as a reference. Also included is information on previous NBS catalogs, and an availability-status table on previously-published papers. A back-edge index permits ready location of the contents.

Those NBS papers that are published by the Government Printing Office are sold by the Superintendent of Documents, and also in microfilm form by the National Technical Information Service (NTIS). These publications listed herein by their respective subject series. NBS-authored papers which appeared in non-NBS publications are cited in a separate numerical sequence.

This catalog, like past supplements, was produced utilizing computer-assisted photocomposition techniques.

W. R. TILLEY, *Chief*  
*Office of Technical Information*  
*and Publications*

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# 1. NBS PUBLICATION PROGRAM

## 1.1. INTRODUCTION

The National Bureau of Standards formal publication program provides a principal and effective means of communicating the results of the Bureau's research, development, and service activities to the scientific and technical community. Publications thus constitute a major end product of the Bureau's efforts, totalling about 900 items per year. These take the form of the Bureau's three periodicals, its ten nonperiodical publications, and articles in the journals of professional organizations and technological associations.

This book, *Publications of the National Bureau of Standards*, lists those publications representing the results of the Bureau's in-house programs; these publications are as follows:

## 1.2. PERIODICALS

### 1.2.1. JOURNAL OF RESEARCH

The *Journal of Research* reports research and development in physics, mathematics, chemistry, and engineering. Comprehensive scientific papers give complete details of the work, including laboratory data, experimental procedures, and theoretical and mathematical analyses. The *Journal* also presents review articles by recognized authorities and compilations of information on subjects closely related to the Bureau's technical program. The *Journal of Research* is issued in two separate sections as follows:

#### A. *Physics and Chemistry*

This section presents papers of interest primarily to scientists working in these fields. It covers a broad range of physical and chemical research, with major emphasis on standards of physical measurements, fundamental constants and properties of matter. Issued six times a year.

Editor: C. W. Beckett

Associate Editor: D. D. Wagman

#### B. *Mathematical Sciences*

This section presents studies and compilations designed mainly for the mathematician and theoretical physicist. Topics in mathematical statistics, theory of experiment design, numerical analysis, theoretical physics and chemistry, logical design and

programming of computers and computer systems are covered, together with short numerical tables. Issued quarterly.

Editor: M. Newman

Associate Editor: F. W. Olver

### 1.2.2. TECHNICAL NEWS BULLETIN

Reports results of Bureau's programs in measurement standards and techniques, properties of matter and materials, engineering standards and services, instrumentation, and automatic data processing.

The best single source of information concerning the Bureau's research, developmental, cooperative and publication activities, this monthly publication is designed for the industry-oriented individual whose daily work involves intimate contact with science and technology—engineers, chemists, physicists, research managers, product-development managers, and company executives. Readers use the *TNB* to learn of new developments with practical applications, to fill in background, to get ideas for further investigations, and for information on NBS services and publications. Issued monthly.

## 1.3. NONPERIODICALS

Ten categories of nonperiodical publications, described as follows, are listed in this catalog:

**MONOGRAPHS**—major contributions to the technical literature on various subjects related to the Bureau's scientific and technical activities.

**HANDBOOKS**—recommended codes of engineering and industrial practice (including safety codes) developed in cooperation with interested industries, professional organizations, and regulatory bodies.

**SPECIAL PUBLICATIONS**—provides material of a particular nature and quality. Includes proceedings of high-level national and international conferences sponsored by NBS, precision measurement and calibration volumes, NBS Research Highlights, and other special publications appropriate to this grouping. This series had previously been designated Miscellaneous Publications.

**APPLIED MATHEMATICS SERIES**—mathematical tables, manuals, and studies.

**NATIONAL STANDARD REFERENCE DATA SERIES**—provides quantitative data on the physical and chemical properties of materials, compiled from the world's literature and critically evaluated. Developed under a world-wide program coordinated by NBS.

**BUILDING SCIENCE SERIES**—research results, test methods, and performance criteria of building materials, components, systems, and structures.

**TECHNICAL NOTES**—designed to supplement the Bureau's regular publications program. Communications and reports of data of limited or transitory interest. Often serve as final reports on work sponsored at NBS by other Government agencies.

**PRODUCT STANDARDS**—developed cooperatively with interested Government and industry groups, and used voluntarily. The term *Product Standards* is now being used to identify all new standards as well as all revisions of existing standards. Existing standards will continue to be referred to as *Commercial Standards or Simplified Practice Recommendations* until such time as they are revised.

**FEDERAL INFORMATION PROCESSING STANDARDS PUBLICATIONS**—publications in this series collectively constitute the Federal Information Processing Standards Register. The purpose of the Register is to serve as the official source of information in the Federal Government regarding (1) uniform Federal information processing standards resulting from provisions of Public Law 89-306 (the Brooks Bill), and (2) data elements and codes standards in data systems developed under the provisions of Bureau of the Budget Circular No. A-86. FIPS PUBS will include approved Federal information processing standards information of general interest, and a complete index of relevant standards publications.

**CONSUMER INFORMATION SERIES**—practical information, based on NBS research and experience, covering areas of interest to the consumer. Easily understandable language and illustrations provide useful background knowledge for shopping in today's technological marketplace.

## 1.4. NBS BIBLIOGRAPHIC SUBSCRIPTION SERVICES

The Cryogenic Data Center and the Electromagnetics Division of the National Bureau of Standards, Boulder, Colorado have developed specialized bibliographic issuances designed to provide interested audiences with information on latest developments in certain specialized fields. These issuances, together with subscription information, are listed below:

### *NBS Bibliographic Subscription Services*

**CRYOGENIC DATA CENTER CURRENT AWARENESS SERVICE** (Publications and Reports of Interest in Cryogenics). A literature survey issued weekly. Annual subscription: Domestic, \$20.00; Foreign, \$25.00.

**LIQUEFIED NATURAL GAS.** A literature survey issued quarterly. Annual subscription: \$20.00.

**SUPERCONDUCTING DEVICES AND MATERIALS.** A literature survey issued quarterly. Annual subscription: \$20.00.

Send subscription orders and remittances for the preceding bibliographic services to the U.S. Department of Commerce, National Technical Information Service, Springfield, Virginia 22151.

**Electromagnetic Metrology Current Awareness Service** (Abstracts of Selected Articles on Measurement Techniques and Standards of Electromagnetic Quantities from D-C to Millimeter-Wave Frequencies). Issued monthly. Annual subscription: \$100.00 (Special rates for multi-subscriptions). Send subscription order and remittance made payable to the Dept. Comm./NBS to the Electromagnetic Metrology Information Center, Electromagnetics Division, National Bureau of Standards, Boulder, Colorado 80302.

## 1.5. PAPERS PUBLISHED BY OTHERS

Many significant contributions by NBS authors are published in other journals. Up-to-date listings of these articles are carried regularly in the Technical News Bulletin, as well as in each section of the Journal of Research, along with selected abstracts.



## 1.6. OSRDB BIBLIOGRAPHY SERIES

Under the National Standard Reference Data System's program administered by the NBS Office of Standard Reference Data (OSRD) each NSRDS data center or compilation project builds up a comprehensive bibliographic file covering its area of interest. This information provides a basis for evaluation and preparation of standard

reference data. It also provides the basis for the OSRDB bibliography series which was inaugurated to make listings of these extensive files available to the technical community. Papers in this bibliographic series are available by purchase from the National Technical Information Service, Springfield, Virginia 22151, see Section 4.1 for a list of these papers.

## 2. PURCHASE PROCEDURES AND DOCUMENT AVAILABILITY

### 2.1. PURCHASE PROCEDURES

The publications of the Bureau are available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, at the prices listed in this publication. You may also order through the U.S. Department of Commerce Field Office nearest you (see page 429 for list of Field Offices of the U.S. Department of Commerce). Nonperiodicals (only) may also be ordered through the National Technical Information Service, U.S. Department of Commerce, Springfield, Virginia 22151.

This section includes price lists of available publications, plus instructions on how to acquire reprints of articles by NBS authors, and how to get out-of-print material.

**How to Make Remittances.** Remittances for publications for which individual sales or subscription prices are shown should be mailed to Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, by coupon, postal money order, express money order, or check. Postage stamps will not be accepted. Publications cannot be mailed before remittances are received. *Foreign remittances should be made either by international money order or draft on an American bank.*

The letter symbol, publication number, and full title of the publication must be given when ordering. The Superintendent of Documents allows a discount of 25 percent on orders of 100 or more copies of one publication.

For the convenience of the general public, coupons in the denomination of five cents may be purchased from the Superintendent of Documents. These may be exchanged for Government publications sold by the Superintendent's office. Address order to Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

Persons who make frequent purchases from the Superintendent of Documents may find a deposit account convenient. Deposits of \$25 or more are accepted against which orders may be placed without making individual remittances or first obtaining quotations. Order blanks are furnished for this purpose. After the order has been processed, the order itself is returned, showing the publications supplied, explanations regarding those not sent, the amount of charge, and the balance on deposit.

No charge is made for postage on documents sent to points in the United States and possessions or to Canada, Mexico, Newfoundland (including Labrador), and certain Central and South American countries. To other countries the regular rate of postage is charged and remittances must cover such postage. In computing foreign postage, add one-fourth of the price of the publication.

Orders for publications purchased from the National Technical Information Service (NTIS) must be accompanied by postal money order, express money order, or check made out to the NTIS and covering total cost of the publications order. Information concerning NTIS coupons can be obtained directly from NTIS. All inquiries or orders should be addressed to: National Technical Information Service, Springfield, Virginia 22151.

### 2.2. ANNOUNCEMENTS OF NBS PUBLICATIONS

The National Bureau of Standards and the agencies mentioned below regularly issue the following official announcements dealing with NBS publications.

**Technical News Bulletin.** Issued monthly by the National Bureau of Standards. In addition to publishing technical news of the

Bureau, the Bulletin announces all new publications by members of the staff whether published in an NBS series or in a non-NBS publication. Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. Annual subscription, \$6.50; \$8.25 foreign. Single copies, 65 cents each.

**Monthly Catalog of United States Government Publications.** Issued monthly by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402. Annual subscription, with consolidated annual index, \$7.00; \$8.75 foreign.

**Price Lists.** These consist of lists of publications prepared by the Superintendent of Documents on special subjects. Single copies sent on request without charge provided you state the subject matter field in which you desire information. For a complete list and order form for subject price lists, request a copy of **How to Keep in Touch with United States Government Publications** from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

**List of Selected Government Publications.** Issued semimonthly by the Superintendent of Documents. Each list is arranged alphabetically by subjects, with annotations and prices. May be obtained free from that office.

**Business Service Check List.** Weekly announcement of publications of the Department of Commerce. Lists titles and prices of National Bureau of Standards Publications, as well as those of other offices of the Department of Commerce. Available from the Superintendent of Documents. Annual subscription, \$2.50; \$4.00 foreign.

## 2.3. CATALOGS OF NBS PUBLICATIONS

Previous catalogs, plus this publication, constitute a complete list of the titles of the Bureau's publications through December 31, 1972. Where the price is given, the catalog is available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C., 20402. Otherwise, it may be consulted in a library which maintains sets of National Bureau of Standards publications.

Circular 460: Publications of the National Bureau of Standards 1901 to June 30, 1947. 375 pages, including subject and author indexes. Brief abstracts are included for the period January 1, 1941 to June 30, 1947 ..... \$1.25

Supplement to Circular 460: Publications of the National Bureau of Standards, July 1, 1947 to June 30, 1957. 373 pages, including subject and author indexes ..... \$1.50

Miscellaneous Publication 240: Publications of the National Bureau of Standards July 1, 1957 to June 30, 1960. First NBS Catalog to Include Titles of Papers Published in Outside Journals 1950 to 1959. 391 pages, including subject and author indexes ..... \$3.50

Supplement to Miscellaneous Publication 240: Publications of the National Bureau of Standards published by NBS, July 1960 through June 1966; published by others, 1960 through 1965. 740 pages, including subject and author indexes ..... \$4.00

Special Publication 305: Publications of the National Bureau of Standards published by NBS. July 1966 through December 1967; published by others, 1966-1967. 223 pages, a citation of titles and abstracts, with key words and author indexes ..... \$2.00

Supplement 1 to Special Publication 305: Publications of the National Bureau of Standards, 1968 through 1969. 497 pages, a citation of titles and abstracts, with key words and author indexes ... \$4.50

Supplement 2 to Special Publication 305: Publications of the National Bureau of Standards, 1970. 378 pages, a citation of titles and abstracts, with key words and author indexes ..... \$3.25

Supplement 3 to Special Publication 305: Publications of the National Bureau of Standards, 1971. 342 pages, a citation of titles and abstracts, with key words and author indexes ..... \$3.00

Supplement 4 to Special Publication 305: Publications of the National Bureau of Standards, 1972, 449 pages, a citation of titles and abstracts, with key words and author indexes ..... \$3.75

## 2.4. FUNCTIONS OF DEPOSITORY LIBRARIES IN THE UNITED STATES

The Superintendent of Documents, United States Government Printing Office, is authorized by law to furnish Government publications to designated depository libraries. The libraries listed in Appendix A are now receiving selected publication series of the National Bureau of Standards for general reference use. Whether a given library has a copy of a particular publication can be determined by inquiring at the library.

## 2.5. FUNCTIONS OF U.S. DEPARTMENT OF COMMERCE FIELD OFFICES

Department of Commerce Field Offices are maintained in the cities listed in Appendix B. Their purpose is to provide ready access, at the local level, to the services of the Department of Commerce as well as to its reports, publications, statistical statements, and surveys. Each Field Office serves as an official sales agent of the Superintendent of Documents, U.S. Government Printing Office, making available for purchase locally a wide range of Government publications. The reference library maintained by each Field



Office contains many Government and private publications, periodicals, directories, reports, and other reference materials.

## 2.6. AVAILABILITY OF NBS PUBLICATIONS

### A. PERIODICAL SUBSCRIPTION RATES

Periodical	Domestic <sup>1</sup>	Foreign <sup>2</sup>
Journal of Research of the National Bureau of Standards:		
Section A. Physics and Chemistry, issued six times a year, paper covers.....	17.00	21.25
Bound volume (1 volume per year), blue buckram .....	( <sup>3</sup> )	( <sup>3</sup> )
Section B. Mathematical Sciences, issued quarterly, paper covers.....	9.00	11.25
Bound volume (1 volume per year), green buckram ( <sup>4</sup> ).....	( <sup>3</sup> )	( <sup>3</sup> )
Technical News Bulletin, 12 monthly issues.....	6.50	8.25

NOTE.—Send order, with remittance, to Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402

<sup>1</sup> United States and its possessions, Canada, Mexico, Newfoundland (including Labrador), and certain Central and South American Countries.

<sup>2</sup> Foreign price includes the cost of the publication and postage.

<sup>3</sup> Prices of the bound volumes vary. The Superintendent of Documents will furnish prices on request.

### B. PRICE LISTS FOR NONPERIODICALS

The following lists give the numbers and prices of all NBS publications issued from 1901 through 1972 which are still in print. Those items in **boldface** denote the 1972 publications cited in this supplement. The prices shown herein supersede prices quoted in previous catalogs of NBS publications. Publications may be ordered from the Superintendent of Documents, U.S. Government Printing Office or from the U.S. Department of Commerce Field Office nearest you. Some NBS publications may be purchased from the National Technical Information Service. (See Section 2.1.)

When an item refers to “see—”, the original item has been superseded by the item referenced, and the price shown is the sales price for the superseding publication. If “OP” is listed instead of a price, that publication is out of print. In such cases, your nearest depository library may still have a copy of the out-of-print item. (See Section 2.4 and Appendix A.)

CIRCULARS (Discontinued Series)

No.	Price	No.	Price	No.	Price
3 see C547, Sec. 1, in part.....	OP	339 see C363.....	OP	500 see TN270-3; 4; 5; and 6	
8 see Mono. 90.....	\$0.25	371 see C378.....	OP	506 see C576.....	*
9 see C602.....	OP	375 see C457.....	OP	508 see C561.....	OP
10 see C425.....	OP	380 see C418.....	OP	510 (PB192339).....	**
12 see C440.....	OP	383 see C424.....	OP	510 Suppl. 1 (PB192340).....	**
16 see C555.....	OP	390 see H71.....	*	510 Suppl. 2 (PB192341).....	**
17 see Mono. 47.....	.30	392 see C432.....	OP	518 see Mono. 70 Vol. I in part (PB168072).....	**
25 see SP260.....	.50	396 see C418.....	OP	533.....	\$2.50
29 see C60.....	OP	398 see SP260.....	\$0.75	536.....	.20
31 see H100.....	.50	399 see C406.....	OP	537 see NSRDS-NBS 10.....	.40
32 see C405.....	OP	400 see C426.....	OP	539 Vol. 1 to 10 are now PB178902 to PB178911.....	**
35 see M183.....	OP	402.....	.10	542 (PB188806).....	**
40 see C381.....	OP	410.....	*	552 see SP260.....	.75
44 see C440.....	OP	413 see C426.....	OP	553.....	2.00
47 see M268.....	.10	414 see H71.....	*	556 (PB172004).....	**
49 see H8.....	OP	415 see Mono. 47.....	.30	559 see H71.....	*
51 see C432.....	OP	428 see C533.....	2.50	563 & 563 Suppl. 1, see M274.....	.50
52 see C387.....	OP	433.....	1.50	564.....	*
54 see H3 & H4.....	OP	434 see C602.....	OP	567 see M271.....	1.25
57 see C410.....	*	435 see H71.....	*	571 (PB175659).....	**
61 see H44, 4th Ed.....	2.00	438.....	*	572 see Mono. 15.....	OP
62 see C424.....	OP	454 (PB192338).....	**	576.....	*
65 see C417.....	OP	450 see C579.....	*	577 & 577 Suppl.....	*
75 see C397.....	OP	456 see Mono. 47.....	.30	579 (PB168350).....	*
76 see C346.....	OP	460.....	1.25	580 see M251.....	OP
82 see C361.....	OP	460 Supplement.....	1.50	582.....	3.25
83 see C333.....	OP	462 see Mono. 80 in part.....	2.75	583 & Suppl. see NSRDS 29.....	.75
95 see C426.....	OP	464.....	*	589 (PB188296).....	**
100 see C592.....	OP	465 see H90 (PB188654).....	**	592 see Mono. 106.....	1.25
101 see C447.....	OP	466 see H71.....	*	593.....	.45
131 see C385.....	OP	467 Vol. I see NSRDS 35 Vol. I.....	5.00	596 (PB172059).....	**
138 see C385.....	OP	467 Vol. II see NSRDS 35 Vol. II.....	4.25	600 see Mono. 90.....	.35
139 see C390.....	OP	467 Vol. III see NSRDS 35 Vol. III.....	4.50	601.....	.30
154 see H71.....	*	470.....	.30	602 (COM 73-10504).....	*
239 see C363.....	OP	474 see C576.....	*		
257 see C365.....	OP	477 see C555.....	OP		
280 see C406.....	OP	478 see Mono. 104.....	.35		
294 see C407.....	OP	482 see C509.....	OP		
300 see C418.....	OP	485 see Mono. 106.....	1.25		
319 see C378.....	OP	495 see Mono. 88.....	.50		
322 see C360.....	OP	499.....	*		
328 see Mono. 15.....	OP				
330 see C362.....	OP				
332 see Mono. 15.....	OP				

\*See page 20 for additional information.

\*\*Available from the National Technical Information Service; use "PB" number when ordering.

# MONOGRAPHS

No.	Price	No.	Price	No.	Price
2 (PB187752).....	*	42 (COM72-10377) .....	*	85 (COM72-10379) .....	*
3 Vol. I (COM71-01000-1).....	*	43 Vol. I.....	*	86 .....	.35
3 Vol. II (COM71-01000-2).....	*	43 Vol. II .....	*	87 .....	.40
4 (PB174987).....	*	44 .....	.15	88.....	\$0.50
7 (COM 73-10503).....	*	45 (PB186433).....	*	89 (AD700466).....	*
8 (PB186237).....	*	46 (PB176590).....	*	90.....	.25
10.....	\$0.20	47 (COM71-00691) .....	*	91.....	2.25
12.....	1.50	49 (COM72-10380) .....	*	92.....	2.75
13 (PB172156).....	*	50 see SP320 .....	1.25	93 (COM 73-10008).....	*
14.....	.15	51 .....	.30	94.....	.75
17.....	.65	52 (COM 73-10500) .....	*	95.....	.45
18 see Mono. 88.....	.50	54 .....	.25	96.....	1.25
20.....	2.75	55 .....	.20	97.....	.25
23 (PB183992).....	*	56 .....	.30	98.....	.55
24.....	.20	57 see M274 .....	.50	99.....	*
25 Sec. 1 (PB178429).....	*	58 (PB193909).....	*	100.....	4.50
25 Sec. 2 (PB178430).....	*	60 .....	.25	101.....	2.75
25 Sec. 3 (PB178431).....	*	62 .....	.15	102.....	.25
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283.....	.35	334 (PB173291).....	*	382.....	*
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307.....	.40	360.....	.50	406.....	.70
308.....	.50	361 Revised 1972.....	1.25	407.....	.40
309.....	.60	362.....	.70	408 see TN482.....	1.25
310.....	.30	363.....	.50	409.....	.40
311.....	.30	364.....	.30	410.....	.25
313.....	.45	365.....	.60	411.....	*
314.....	.55	365-1.....	1.00	412.....	.15
315.....	.25	366.....	1.25	413.....	.30
316.....	.35	367.....	.60	414 (PB176109).....	*
318.....	.55	368.....	.25	415.....	.50
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420.....	.15	473.....	.25	519.....	.50
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427.....	.45	479.....	.75	525.....	.75
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431.....	.30	481.....	.30	527.....	.60
432.....	.65	482 see TN 724.....	1.00	528.....	.60
433.....	.25	483.....	.30	529.....	.30
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435.....	.15	485.....	.35	531.....	.70
436.....	.30	486.....	.35	532.....	.45
437.....	.25	487.....	.30	533.....	1.00
438.....	.70	488.....	.50	534.....	.50
439.....	*	489.....	.60	535.....	1.75
440.....	.40	490.....	.30	536.....	.35
441 see TN526.....	1.25	491.....	.25	537.....	.30
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444.....	*	496.....	.60	541.....	.65
445.....	.35	497.....	.30	542.....	1.25
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448.....	.70	498-2.....	.45	545.....	1.25
449.....	.30	499.....	.65	546.....	1.25
451.....	1.25	500.....	.60	547.....	1.25
452.....	1.00	501.....	1.25	548.....	1.25
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454.....	.55	503.....	1.00	550.....	.50
455.....	1.25	504.....	\$1.00	551.....	1.50
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458.....	1.00	507.....	1.25	554.....	1.50
459.....	.60	508.....	1.25	555.....	.65
461.....	.50	509.....	.70	556 (COM 71-50062).....	*
462.....	.65	510.....	.50	557.....	.35
463.....	1.25	511.....	.30	558.....	.50
464.....	1.25	512.....	.25	559.....	1.50
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566.....	.20			712.....	.25
567.....	.70	602.....	.30	713.....	.30
568.....	.70	603.....	1.00		
569.....	.70	604.....	.35	714.....	1.00
570.....	.25	605.....	1.25	715.....	1.00
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571.....	.60			717.....	.55
572.....	.35			718.....	.40
573.....	.35	607.....	.65		
574.....	.50	608.....	.35	719.....	.55
575.....	.45	609.....	.75	720.....	.35
		610.....	1.50	721.....	1.50
576.....	.45	611.....	.35	722.....	.60
577.....	.55			723.....	.45
578.....	.35	612.....	.35		
579.....	.20	613.....	.40	724.....	1.00
580.....		614.....	.50	725.....	.50
		615.....	1.25	726.....	1.25
581.....		616.....	.70	727.....	.70
582.....	1.25			728.....	.70
583.....		617.....	1.50		
584.....	1.50	618.....	.75	729.....	.60
585.....	.70	619.....	1.50	730.....	.35
		621.....	.65	731.....	.60
586.....		622.....	1.25	732.....	.45
587.....	1.25			733.....	.60
588.....					
589.....	.60	623.....	.35	734.....	.35
590 (COM 71-50292).....	*	624.....	1.00	735.....	.40
		699.....		736.....	.50
591.....	.50	700.....	.75	737.....	2.25
592.....	.70	702.....	.50	738.....	.25
593.....	.60				
594-1.....	.60	703.....	.50	739.....	.35
594-2.....	.50	706.....	.25	742.....	.60
		707.....	.30	743.....	1.00
594-3.....	.60	708 (COM 72-50062).....	*	744.....	.55
595.....	.65	709.....	.30	746.....	2.00
596.....	.65	710-1.....	.25	747.....	1.25
597.....	.50	710-2.....	.35	749.....	1.50
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issued a publication on this subject. Listed as ASTM D900-55, it can be ordered at 75 cents per copy.

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*Miscellaneous Publication 179, American Standard Building Code Requirements for Minimum Design Loads in Buildings and Other Structures.* The American National Standards Institute, 1430 Broadway, New York, N.Y. 10018, has issued a publication on this subject. Available from them as A58.1-1969, at \$2.75.

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*Handbook 102, ASTM Metric Practice Guide.* American Society for Testing and Materials,

1916 Race Street, Philadelphia, Pa. 19103, has issued a publication as Document E380-72, at \$1.50.

*Handbook 110-1, National Electrical Safety Code.* Part 1. Rules for the Installation and Maintenance of Electrical Supply Stations and Equipment (C2.1-1971) is available from the American National Standards Institute, 1430 Broadway, New York, N.Y. 10018, at \$1.50. C2.3- Safety Rules for the Installation and Maintenance of Underground Electric Supply and Communication Lines and C2.4- Rules for the Operation of Electric Supply and Communication Lines and Equipment are in press and will be available from the above address.



### 3. TITLES AND ABSTRACTS OF NBS PUBLICATIONS, 1972<sup>1</sup>

#### 3.1. PAPERS FROM THE JOURNAL OF RESEARCH OF THE NATIONAL BUREAU OF STANDARDS, SECTION A. PHYSICS AND CHEMISTRY, VOLUME 76A, JANUARY-DECEMBER 1972

##### January-February 1972

The absorption spectra of krypton and xenon in the wavelength range 330-600 Å, K. Codling and R. P. Madden, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 1, 1-12 (Jan.-Feb. 1972).

Key words: Autoionization; far ultraviolet; krypton; photoionization; resonances; xenon.

A total of 153 krypton resonances in the spectral region 330-500 Å and 253 xenon resonances in the spectral region 375-600 Å are reported. A detailed listing of the resonances is given, with wavelength and line shape information. The analysis of the spectra is very incomplete and will require detailed theoretical calculation to significantly improve it. In Kr, 45 resonances and in Xe, 56 resonances have been grouped into probable Rydberg series, for which classifications are suggested. The resonances are due, in the main, to either the excitation of the inner subshell "s" electron ( $s^2p^6 \rightarrow sp^6np$ ) or to the excitation of two of the outer "p" electrons simultaneously ( $s^2p^6 \rightarrow s^2p^4nln'l'$ ). These high-lying excited states autoionize, resulting in resonances with window-, asymmetric-, or absorption-type profiles. Where possible, comparisons are made with previous work.

A reference calorimeter for laser energy measurements, E. D. West, W. E. Case, A. L. Rasmussen, and L. B. Schmidt, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 1, 13-26 (Jan.-Feb. 1972).

Key words: Calorimetry; laser; laser calorimetry; laser energy measurement; laser power measurement.

Principles and detailed procedures are described for measuring laser energy and power in terms of electrical energy based on voltage, resistance, and frequency standards. The construction of a small isoperibol calorimeter used for the measurements is described. The calorimeter will accommodate 0.01 to 20 J and  $4 \times 10^{-5}$  to 1 W cw and is limited to a maximum pulse intensity of 0.1 J/cm<sup>2</sup>. The standard deviation of comparison measurements using two calorimeters and a beam splitter is 0.08 percent when the smaller energy input is not less than 0.3 J. The estimated limits of systematic error for one calorimeter are  $\pm 1.0$  percent of the laser energy measured by the calorimeter.

Accurate calculations of properties of the two-tube electrostatic lens. I. Improved digital methods for the precise calculation of electric fields and trajectories, S. Natali, D. Di Chio, and C. E. Kuyatt, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 1, 27-35 (Jan.-Feb. 1972).

Key words: Calculation of electric fields; calculation of electron trajectories; electron lens; nine-point relaxation

formulas; predictor-corrector method; two-tube electrostatic lens.

Digital methods of high precision have been developed for the calculation of electric fields and trajectories in electrostatic lenses and a computer program was written to apply these methods to the two-tube lens. The increased precision results from the use of nine-point formulas in the relaxation calculation of potentials in place of previously used five-point formulas and from the use of an improved predictor-corrector method for the calculation of trajectories. Trajectories obtained with these methods are sufficiently precise to determine third-order aberration coefficients.

Dielectric constant of compressed gaseous and liquid oxygen, B. A. Younglove, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 1, 37-40 (Jan.-Feb. 1972).

Key words: Clausius-Mossotti function; dielectric constant; oxygen.

The dielectric constants of compressed gaseous and liquid oxygen were measured on ten isotherms at temperatures between 100 and 300 K and on the saturated liquid boundary at temperatures between 55 and 154 K. Densities ranged from 0.06 to 1.30 g/cm<sup>3</sup> at pressures up to 33 MN/m<sup>2</sup>. The dielectric constant measurements were combined with accurate density data to compute the Clausius-Mossotti (CM) function,  $(\epsilon - 1)/(\epsilon + 2)\rho$ . The CM function for oxygen decreases with density from a value of 0.1236 cm<sup>3</sup>/g at the low density limit to 0.1219 cm<sup>3</sup>/g near the triple point.

Thermal analysis of calcium sulfate dihydrate and supposed  $\alpha$  and  $\beta$  forms of calcium sulfate hemihydrate from 25 to 500 °C, J. R. Clifton, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 1, 41-49 (Jan.-Feb. 1972).

Key words:  $\alpha$ - and  $\beta$ -CaSO<sub>4</sub> · 1/2H<sub>2</sub>O; CaSO<sub>4</sub> · 2H<sub>2</sub>O; differential scanning calorimetry; differential thermal analysis; thermogravimetry.

Thermal studies were carried out on CaSO<sub>4</sub> · 2H<sub>2</sub>O and the supposed  $\alpha$  and  $\beta$  forms of CaSO<sub>4</sub> · 1/2H<sub>2</sub>O in the region of 25 to 500 °C using differential thermal analysis, thermogravimetry, and differential scanning calorimetry methods.

Two large endothermic effects and a smaller exothermic effect were found in the differential thermogram of CaSO<sub>4</sub> · 2H<sub>2</sub>O while a single endothermic as well as an exothermic effect were found in the thermograms of the supposed  $\alpha$  and  $\beta$  forms of CaSO<sub>4</sub> · 1/2H<sub>2</sub>O. However, the exotherm of  $\alpha$ -CaSO<sub>4</sub> · 1/2H<sub>2</sub>O had lower peak and first-break temperatures than that of the  $\beta$ -form. The peak and first-break temperatures of the endothermic effects of CaSO<sub>4</sub> · 2H<sub>2</sub>O and  $\alpha$  and  $\beta$ -CaSO<sub>4</sub> · 1/2H<sub>2</sub>O and the exothermic effect of  $\alpha$ -CaSO<sub>4</sub> · 1/2H<sub>2</sub>O were pressure dependent, shifting to lower temperatures as the gaseous pressure within the DTA cell was decreased. The noted differences in the thermograms possibly are due to kinetic factors because of the differences in crystallinity of the supposed  $\alpha$ - and  $\beta$ -CaSO<sub>4</sub> · 1/2H<sub>2</sub>O.

<sup>1</sup> The various NBS publications series are grouped under subheadings within this section. The several volumes of the Journal of Research are presented consecutively within their appropriate subheadings. If a particular publications series is sought, consult the table of contents or the edge index on the back cover.



No differences in the supposed  $\alpha$  and  $\beta$  forms of  $\text{CaSO}_4 \cdot 1/2\text{H}_2\text{O}$  were detected by thermogravimetry and differential scanning calorimetry studies. The formulation of a two-step dissociative process in the complete dehydration of  $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$  was supported by the results of the thermogravimetry study.

#### Modulus of natural rubber cross-linked by dicumyl peroxide. I.

Experimental observations, L. A. Wood, G. W. Bullman, and G. E. Decker, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 1, 51-59 (Jan.-Feb. 1972).

Key words: Creep; cross-linking; dicumyl peroxide; glass transition; indentation measurements; rubber, natural.

Natural rubber mixed with varying amounts of dicumyl peroxide was cross-linked by heating 120 min at 149 °C. The quantitative measure of cross-linking was taken as the amount  $fp$  of decomposed dicumyl peroxide, the product of  $p$ , the number of parts added per hundred of rubber and  $f$  the fraction decomposed during the time of cure. The shear creep modulus  $G$  was calculated from measurements of the indentation of a flat rubber sheet by a rigid sphere. The glass transition temperature  $T_g$ , was raised about 1.2 °C for each part of decomposed dicumyl peroxide. Above  $(T_g + 12)$  the modulus-temperature relations were linear with a slope that increased with increasing cross-linking. The creep rate was negligible except near the glass transition and at low values of  $fp$ . Values of  $G$ , read from these plots at seven temperatures, were plotted as a function of  $fp$ . The linearity of the two plots permits the derivation of the general relation:  $G = S(fp + B)T + H(fp + B) + A$  where  $A$ ,  $B$ ,  $H$ , and  $S$  are constants. The lines representing  $G$  as a function of  $fp$  at each temperature all intersected near the point,  $fp = 0.45$  phr,  $G = 2.70$  Mdyn  $\text{cm}^{-2}$  (0.270 MN  $\text{m}^{-2}$ ). The constants were evaluated as  $A = 2.70$  Mdyn  $\text{cm}^{-2}$ ,  $B = -0.45$  phr,  $S = 5.925 \times 10^{-3}$  Mdyn  $\text{cm}^{-2}$  (phr) $^{-1}\text{K}^{-1}$  and  $H = 0.0684$  (Mdyn  $\text{cm}^{-2}$ ) (phr) $^{-1}$ . This equation represented satisfactorily all the data obtained at temperatures from  $-50$  to  $+100$  °C for values of  $fp$  from about 1 to 24 phr.

### March-April 1972

Guidelines for the reporting of numerical data and experimental procedures, D. Garvin, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 2, 67-70 (Mar.-Apr. 1972).

Key words: Chemistry; experimental procedures; numerical data; physics.

General recommendations are made about the reporting of data and experimental procedures. These are intended as instructions to authors of papers in which quantitative physical and chemical data are reported. There is included a bibliography of standards documents and more detailed guidelines.

A study of equilibrium in argon arcs, J. B. Shumaker and C. H. Popenoe, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 2, 71-76 (Mar.-Apr. 1972).

Key words: Argon arcs; argon transition probabilities; equilibrium; LTE.

The intensities of the 7147 Å Ar I and 4806 Å Ar II lines obtained from wall-stabilized arcs at pressures of 0.2 to 5 atm are presented in an Olsen-Richter diagram. Departures from equilibrium are evident at electron densities below  $5 \times 10^{16} \text{ cm}^{-3}$ . The assumption of equilibrium at higher electron densities leads to transition probabilities in fair agreement with lifetime measurements.

Rates of reaction of atomic oxygen III. Spiropentane, cyclopentane, cyclohexane, and cycloheptane, R. E. Huie and J. T. Herron, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 2, 77-80 (Mar.-Apr. 1972).

Key words: Cycloheptane; cyclohexane; cyclopentane; oxygen; rate constants; spiropentane.

Rate constants have been measured from 307 to 652 K for the reactions of atomic oxygen ( $\text{O}^3\text{P}$ ) with spiropentane, cyclopentane, cyclohexane, and cycloheptane. The derived Arrhenius parameters are  $k(\text{sp} - \text{C}_5\text{H}_8) = 10^{13.60 \pm 0.10} \exp[(-2890 \pm 100)/T]$ ,  $k(\text{cy} - \text{C}_5\text{H}_{10}) = 10^{14.10 \pm 0.09} \exp[(-2210 \pm 100)/T]$ ,  $k(\text{cy} - \text{C}_6\text{H}_{12}) = 10^{14.35 \pm 0.09} \exp[(-2350 \pm 100)/T]$ , and  $k(\text{cy} - \text{C}_7\text{H}_{14}) = 10^{14.46 \pm 0.13} \exp[(-2230 \pm 100)/T]$  all in units of  $\text{cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ .

Densities of compressed liquid methane, and the equation of state, R. D. Goodwin and R. Prydz, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 2, 81-101 (Mar.-Apr. 1972).

Key words: Compressed liquid; densities; equation of state; methane; orthobaric densities.

Experimental PVT data for liquid methane are reported at densities from 1.8 times critical up to the freezing liquid, at temperatures from 91 to 245 K and pressures to 350 bar. A nonanalytic equation of state is adjusted to these and other PVT data from ideal gas states to the freezing liquid, at temperatures from the triple point to 400 K.

Spin-relaxation effects on the EPR spectrum of gaseous hydrogen atoms, R. L. Brown, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 2, 103-113 (Mar.-Apr. 1972).

Key words: Electron spin resonance; hydrogen atoms; spin-exchange; spin-relaxation.

A theoretical analysis is presented of the relaxation processes which lead to the magnetization of gaseous hydrogen atoms in a strong magnetic field. Experiments are described which demonstrate that the spin-lattice relaxation time in a pure  $\text{H}_2$  carrier can be of the order of 10 ms. From the effects of traces of  $\text{O}_2$  on the hydrogen atom EPR spectrum, a  $\text{H}-\text{O}_2$  spin-exchange collision cross section of  $(8.0 \pm 2.5) \times 10^{-16} \text{ cm}^2$  was derived.

Photoionization of  $\text{C}_4\text{H}_8^+$  isomers. Unimolecular and bimolecular reactions of the  $\text{C}_4\text{H}_8^+$  ions, L. W. Sieck, S. G. Lias, L. Hellner, and P. Ausloos, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 2, 115-124 (Mar.-Apr. 1972).

Key words:  $\text{C}_4\text{H}_8$  isomers; collisional stabilization; isomerization; photoionization; rate constants; vapor phase.

1-Butene, *cis*-2-butene, isobutene and methylcyclopropane have been photoionized with the resonance lines of krypton (10.0 – 10.6 eV) and argon (11.6 – 11.8 eV). We have determined that the internally excited  $1-\text{C}_4\text{H}_8^+$  ion and, to a much lesser extent, the  $i-\text{C}_4\text{H}_8^+$  ion isomerizes to the  $2-\text{C}_4\text{H}_8^+$  structure. In both cases the extent of isomerization increases, approximately by a factor of ten when the photon energy is increased from 10 to 11.7 eV. An inert gas, neon, quenches the isomerization of the  $i-\text{C}_4\text{H}_8^+$  ion and, to a much lesser extent, that of the  $1-\text{C}_4\text{H}_8^+$  ion.

The unimolecular fragmentation of the  $\text{C}_4\text{H}_8^+$  isomeric ions has been examined at 11.6 – 11.8 eV. In this energy range the dissociative lifetime of  $i-\text{C}_4\text{H}_8^+$  was found to be at least  $5 \times 10^{-6}$  s, and collisional quenching of the dissociative process is already noticeable at pressures in the  $10^{-3}$  torr range.

The rate coefficients for the reaction  $\text{C}_4\text{H}_8^+ (\text{thermal}) + \text{C}_4\text{H}_8 \rightarrow (\text{C}_8\text{H}_{16}^+)^*$  occurring in the isomeric  $\text{C}_4\text{H}_8$  systems have been determined under conditions where the structure of the reacting  $\text{C}_4\text{H}_8^+$  ion is established. The values in  $\text{cm}^3/\text{molecule} \cdot \text{second}$  are  $1-\text{C}_4\text{H}_8 - 6.0 \pm 0.5 \times 10^{-10}$ , *cis*-2- $\text{C}_4\text{H}_8 - 0.37 \pm 0.1 \times 10^{-10}$ ,  $i-\text{C}_4\text{H}_8 - 5.4 \pm 0.4 \times 10^{-10}$ . At pressure below  $10^{-3}$  torr, the internally excited  $(\text{C}_8\text{H}_{16}^+)^*$  produced in the reaction dissociates along various channels with relative probabilities de-

pending upon the structure of both the ionic and neutral reactant. Above  $10^{-3}$  torr collisional quenching of  $(C_8H_{16}^+)^*$  is noted.

**Theoretical investigation of the odd configurations of Ni II, Y. Shadmi and E. Caspi, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 125-136 (Mar.-Apr. 1972).**

Key words: Energy levels;  $g$ -factors; nickel; parameters; theory.

Two groups of odd levels in Ni II were investigated: those belonging to the complex  $3d^8 4p + 3d^7 4s 4p + 3d^6 5p$  and those belonging to the configuration of  $3d^8 4f$ . In the first group the calculated positions of the levels were fit to the positions of the 174 observed levels with an rms error of  $133\text{ cm}^{-1}$ . The fit for the second group was based on 60 observed levels and had an rms error of  $25\text{ cm}^{-1}$ . The predictions of this investigation helped in the discovery of many of the observed levels.

**The characterization of linear polyethylene SRM 1475. I. Introduction, C. A. J. Hoeve, H. L. Wagner, and P. H. Verdier, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 137-138 (Mar.-Apr. 1972).**

Key words: Fractionation; linear polyethylene; molecular weight; molecular weight distribution; National Bureau of Standards; pellet variability; standard reference material.

The National Bureau of Standards has issued a linear polyethylene standard reference material, SRM 1475. In this report a general description of the sample is given, and the characterization work described in the subsequent reports is outlined. Some pellet-to-pellet variability was found and estimated.

**The characterization of linear polyethylene SRM 1475. II. Determination of total methyl content by infrared spectrophotometry, J. E. Brown, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 141-142 (Mar.-Apr. 1972).**

Key words: Infrared; linear polyethylene; methyl; methylene; number average molecular weight; spectra; spectrophotometry.

An ASTM method was used to determine the methyl content of linear polyethylene SRM 1475 by measuring the absorbance at  $1378\text{ cm}^{-1}$  ( $7.25\text{ nm}$ ) of methyl groups on compensated infrared spectra. The methyl content of this polymer was found to be 0.15 methyls per 100 carbon atoms. Considering the methyls to be polymer end groups, the number average molecular weight computed approximates that determined by gel permeation chromatography within the experimental error. These values indicate that the polymer is essentially free of branching.

**The characterization of linear polyethylene SRM 1475. III. Density determination, J. E. Brown, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 143-144 (Mar.-Apr. 1972).**

Key words: Crystallization; degree of crystallinity; density; linear polyethylene; polymer; recrystallization.

The density of SRM 1475 at  $23^\circ\text{C}$  was determined by ASTM method D 1505-67 on samples prepared by Procedure A of ASTM method D 1928-68, with the result  $0.9784\text{ g/cm}^3$ .

**The characterization of linear polyethylene SRM 1475. IV. Melt flow rate, J. R. Maurey, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 145-146 (Mar.-Apr. 1972).**

Key words: Extrusion plastometer; load; melt flow rate; orifice; orifice die; preliminary extrudate; test extrudate.

The melt flow rate of SRM 1475 was determined to be  $2.07\text{ g/10 min}$  at  $190^\circ\text{C}$  under a load of  $325\text{ g}$  by a method similar to procedure A of ASTM method D 1238-65T. This value is the average of determinations on 42 samples with a standard deviation

of a single measurement of  $0.040\text{ g/10 min}$ , and a range of  $1.991\text{ g/10 min}$  to  $2.132\text{ g/10 min}$ .

**The characterization of linear polyethylene SRM 1475. V. Solution viscosity measurements, R. G. Christensen, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 147-149 (Mar.-Apr. 1972).**

Key words: Decalin; limiting viscosity number; linear polyethylene; solution viscosity; viscometer; 1-chloronaphthalene; 1,2,4-trichlorobenzene.

The limiting viscosity numbers of linear polyethylene SRM 1475 were determined at  $130^\circ\text{C}$  in 1,2,4-trichlorobenzene, 1-chloronaphthalene, and decalin. Technique, including use of a novel solution transfer method, is described.

**The characterization of linear polyethylene SRM 1475. VI. Preparation of calibrating fractions, R. G. Christensen, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 149-150 (Mar.-Apr. 1972).**

Key words: Column extraction fractionation; fractionation; linear polyethylene.

Fractions for use in calibrating a gel permeation chromatograph were prepared by a Desreux column extraction method. The construction and operation of the fractionating system are described.

**The characterization of linear polyethylene SRM 1475. VII. Differential refractive index of polyethylene solutions, H. L. Wagner, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 151-155 (Mar.-Apr. 1972).**

Key words: Differential refractive index;  $dn/dc$ ; refractive index; refractometer; 1-chloronaphthalene; 1,2,4-trichlorobenzene.

The value of  $dn/dc$  for polyethylene in 1-chloronaphthalene at  $135^\circ\text{C}$ , required for the determination of molecular weight by light scattering, was found to vary with molecular weight. Similar changes were found in 1,2,4-trichlorobenzene, the gel permeation chromatograph solvent. The absolute value of  $dn/dc$  decreases by about 2 percent as the polymer molecular weight increases from 12,000 to 110,000.

**The characterization of linear polyethylene SRM 1475. VIII. Light-scattering studies on polyethylenes in 1-chloronaphthalene, L. J. Frolen, G. S. Ross, A. M. Wims, and P. H. Verdier, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 156-160 (Mar.-Apr. 1972).**

Key words: End-to-end distance; light scattering; linear polyethylene;  $M_w$ ; polyethylene fractions; second virial coefficient; solution properties.

Light-scattering measurements have been made on a series of linear polyethylene fractions and a linear polyethylene standard reference material (SRM 1475). All measurements were made in 1-chloronaphthalene at  $135^\circ\text{C}$ , and over an angular range from  $45$  to  $135^\circ$ . The data were analyzed to obtain the weight average molecular weights, second virial coefficients and root-mean square end-to-end distances.

**The characterization of linear polyethylene SRM 1475. IX. Number average molecular weight of fractions by membrane osmometry, J. E. Brown and P. H. Verdier, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 2, 161-163 (Mar.-Apr. 1972).**

Key words: Concentration dependence; linear polyethylene; membrane; number average molecular weight; osmometer; osmotic pressure; virial coefficient.



The number average molecular weights of a series of fractions of linear polyethylene have been determined using a high speed membrane osmometer. The  $M_n$  values of the fractions, which were prepared by an elution technique, were used in GPC calibration and subsequent characterization of linear polyethylene SRM 1475. The molecular weights, measurement techniques, and the precision of the measurements are presented.

**The characterization of linear polyethylene SRM 1475. X. Gel permeation chromatography,** G. Ross and L. Frolen, *J. Res. Nat. Bur. Stand. (U.S.),* 76A (Phys. and Chem.), No. 2, 163-170 (Mar.-Apr. 1972).

**Key words:** Gel permeation chromatography (GPC); linear polyethylene; molecular weight distribution (MWD); number average; weight average.

The determination of the integral molecular weight distribution (MWD) of the linear polyethylene sample (SRM 1475) by means of gel permeation chromatography (GPC) is described. Both the experimental and mathematical details of column calibration and sample analysis are included.

## May-June 1972

**Thermodynamics of standard cells of the saturated cadmium sulfate type,** W. J. Hamer, *J. Res. Nat. Bur. Stand. (U.S.),* 76A (Phys. and Chem.), No. 3, 185-205 (May-June 1972).

**Key words:** Emfs of standard cells; emf-temperature coefficients of standard cells; standard potential of standard cells; thermodynamics of standard cells.

This paper gives data on the thermodynamic functions of standard cells of the saturated cadmium sulfate type, as obtained from calorimetric and equilibrium data at 25 °C or from the electromotive forces (emfs) and emf-temperature coefficients of the cell for the temperature range of 0 to 43.6 °C. The functions considered are the changes in Gibbs energy, enthalpy, entropy and heat capacity for the cell reaction. The electromotive forces are expressed on the  $V_{69}$  volt and the  $t_{69}$  temperature scale. Results are expressed on the S1 and for comparisons with literature data in terms of the defined thermochemical calorie. The effect of expressing the emf-temperature coefficient as a function of temperature in different ways on the values for the changes in entropy and heat capacity for the cell reaction is discussed. Finally, the observed emf of the standard cell at 25 °C is compared with emfs calculated from various values reported for the standard potentials of the cadmium-amalgam and mercury-mercurous sulfate electrodes and the activity coefficient of cadmium sulfate in saturated aqueous solution.

**An improved state equation in the vicinity of the critical point,** O. B. Verbeke, *J. Res. Nat. Bur. Stand. (U.S.),* 76A (Phys. and Chem.), No. 3, 207-211 (May-June 1972).

**Key words:** Compressibility; critical point; equation of state; fluid; helium; low temperature; methane; scaling law; specific heat; xenon.

An improved state equation for the vicinity of the critical point is proposed. An analysis of the experimental data on helium and xenon has been carried out in order to investigate the influence of the number of constants in the equation and the  $P\rho T$  range on the critical constants  $T_c$  and  $\rho_c$  and on the critical exponents  $\alpha$ ,  $\beta$ ,  $\gamma$ , and  $\delta$ . No such influence has been detected. The model for the critical point, recently proposed by Widom, has been checked regarding its consequences for the rectilinear diameter. No definite confirmation but indications for its correctness have been found.

**Dilute solution theory of polymer crystal growth: fractionation effects,** I. C. Sanchez and E. A. DiMarzio, *J. Res. Nat. Bur. Stand. (U.S.),* 76A (Phys. and Chem.), No. 3, 213-223 (May-June 1972).

**Key words:** Cilia; dissolution temperature; fractionation; rate constant; undercooling.

A nonequilibrium (kinetic) theory of polymer molecular weight (MW) fractionation is formulated and applied to binary and multicomponent polyethylenes crystallized from unstirred xylene solutions. High MW components crystallize more readily than do low MW components. This fractionation effect is enhanced as the crystallization temperature is raised. At low crystallization temperatures (high undercoolings) the polymer tends to fractionate according to the volume fraction distribution of its MW components and thus, the number average MW of the crystal that is formed is approximately equal to the weight average MW of the polymer in solution. It is shown that MW fractionation does not depend on the details of nucleation, but rather on the rates for post-nucleation crystal growth. The effects of MW polydispersity on crystalline properties is considered and in particular it is shown that polydispersity tends to mask the intrinsic dependence of crystal thickness on MW. The variables which govern and influence fractionation are also discussed.

**The formation of curved polymer crystals: poly(4-methylpentene-1),** F. Khoury and J. D. Barnes, *J. Res. Nat. Bur. Stand. (U.S.),* 76A (Phys. and Chem.), No. 3, 225-252 (May-June 1972).

**Key words:** Chain-folded; crystal, curved; electron microscopy; lamellar; optical microscopy; poly(4-methylpentene-1); polymer; solution-grown.

An optical and electron microscopical study is described of the habits exhibited by poly(4-methylpentene-1) crystals (Modification 1 tetragonal unit cell) grown at temperatures between 50 and 90 °C from 0.1 percent solutions of the polymer in equimolar mixtures of xylene and amyl acetate. A distinct trend in the effect of crystallization temperature (supercooling) on the habits of the crystals is illustrated and discussed. The lamellar crystals formed in that temperature range are all the more pronouncedly curved the lower the crystallization temperature. To indicate but the extremes in this trend, the crystals varied from essentially planar ones whose constituent square shaped chain-folded lamellae (bounded laterally by {100} faces and up to 20  $\mu\text{m}$  on a side) are four-sectored and only very slightly buckled as previously indicated by Bassett et al., to distinctly curved four-fold symmetrical hollow bowl shaped ones having a radius of curvature of about 2.5  $\mu\text{m}$  and in which the surface of the curved multilayered wall of which they are constituted changes in orientation through 180° from the base (pole) to the periphery. In contrast with the four-sectored character of the lamellae in the aforementioned essentially planar crystals, the constituent lamellae in all the distinctly dishd and bowl-like crystals formed in the temperature range 50 to 90 °C are multisectored, their lateral development being characterized by the formation at their periphery during growth of successive arrays of {100} microfaceted sectored outgrowths. The reasons why the lamellar crystals of poly(4-methylpentene-1) are all the more pronouncedly curved the lower the crystallization temperature are explored and discussed. Conjectures concerning the origins of this phenomena are advanced in the form of a working "model."

**Photoionization of propylene, cyclopropane, and ethylene. The effect of internal energy on the bimolecular reactions of  $\text{C}_2\text{H}_4^+$  and  $\text{C}_3\text{H}_6^+$ ,** L. W. Sieck and P. Ausloos, *J. Res. Nat. Bur. Stand. (U.S.),* 76A (Phys. and Chem.), No. 3, 253-262 (May-June 1972).



**Key words:** Collisional stabilization; hydrocarbons; ion-molecule reactions; photoionization; rate constants; structures of ions.

The ion-molecule chemistry occurring in photoionized ethylene, propylene and cyclopropane has been investigated in the NBS high pressure mass spectrometer. Emphasis has been placed on determining the overall effect of internal excitation on the absolute rate coefficients for the various reactions. This was accomplished by comparing the behavior found when ionization was induced by photon absorption at the ionization threshold with that found at higher photon energies. The values for the absolute rate coefficients for the formation of excited compound ions at various photon energies were as follows (units of  $10^{-10}$  cm<sup>3</sup>/molecule · s):  $C_2H_4^+$ , 9.6 (10.6 eV photons); 8.5 (11.7 eV photons);  $C_3H_6^+$ , 8.4 (10.0 eV photons); 6.8 (11.7 eV photons);  $C_3D_6^+$ , 7.8 (10.0 eV photons); 6.1 (11.7 eV photons);  $c-C_3H_6^+$  and  $c-C_3D_6^+$ , 2.2 (10.0 eV photons); 2.2 (11.7 eV photons). The distributions of product ions obtained from the unimolecular decomposition of the compound ion in each system have also been determined at various photon energies, and considerable variation has been observed. In general, the variations are similar to those found elsewhere when the kinetic energy of the reactant ion is increased. The bimolecular reactions of the  $C_6D_{12}^+$  compound ion obtained from  $C_3D_6^+$  have been investigated at higher pressures, and separate experiments involving isotopically labeled ethylenes have provided new information concerning the nature of the compound ion in that system. Results obtained from other laboratories are discussed in some detail, and in most cases the differences found for the same system are explicable in terms of the energy content (internal and/or kinetic) of the reactant ion.

**Low temperature thermocouples: KP, "normal" silver, and copper versus Au-0.02 at% Fe and Au-0.07 at% Fe, L. L. Sparks and R. L. Powell, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 3, 263-283 (May-June 1972).**

**Key words:** Cryogenics; gold alloy; liquid helium; liquid hydrogen; liquid nitrogen; thermocouples.

The Seebeck thermoelectric voltages of two dilute alloys of iron in gold, Au 0.02 at% Fe and Au-0.07 at% Fe, have been determined with respect to KP (a particular Ni-Cr alloy), "normal" silver, and copper in the temperature range from 4 to 280 K. The power series representation of these data, along with the calculated Seebeck coefficients and derivatives of the Seebeck coefficients, have been extrapolated to 0 K and are presented as a function of temperature. In addition to these reference data, seven different Au-0.07 at% Fe alloys were thermoelectrically intercompared in order to determine the variability in wires from different melts and from different manufacturers. The largest deviation found amounted to about 9 percent of the output of a KP versus Au-0.07 at% Fe thermocouple pair between 4 and 20 K. A more typical variation for this temperature range was 2 to 4 percent. Initial indications are that the reference data can be adjusted satisfactorily with data from spot calibrations on particular wires. The effect of heat treatment is illustrated by comparing our results to Rosenbaum's data for annealed and unannealed specimens of both Au-Fe alloys.

**Infrared spectra of cerium (Ce I and Ce II) between 0.8 and 2.4  $\mu$ m, J. Verges, C. H. Corliss, and W. C. Martin, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 3, 285-304 (May-June 1972).**

**Key words:** Ce I and II; cerium spectra; infrared spectra; spectra; wavelengths.

The cerium spectrum emitted by an electrodeless lamp has been observed with a SISAM spectrometer in the region from 0.82 to 2.42  $\mu$ m. Of the 2076 lines observed, about 1100 lines

have been classified as transitions in the energy level system of Ce I and 400 lines in Ce II. The average deviation between the observed wave numbers and those calculated from the two energy levels is  $\pm 0.023$  cm<sup>-1</sup>.

## July-August 1972

**The EMF-temperature coefficient of "acid" standard cells of the saturated cadmium sulfate type from 15 to 40 °C, W. J. Hamer, A. Skapars, and B. F. Field, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 4, 321-328 (July-Aug. 1972).**

**Key words:** Effect of acid on standard cells; EMF-temperature coefficients of standard cells; entropy changes in standard cells; heat-capacity changes in standard cells; standard cells.

This paper gives the results of new measurements of the effect of temperature on the electromotive force of standard cells of the saturated cadmium sulfate type. Measurements were made over the temperature range of 15 to 40 °C. Twelve cells of NBS manufacture and 24 cells supplied by two different commercial manufacturers were used in the studies. Final results were analyzed by the method of least squares using computer programs. The relation between EMF and temperature for NBS, company 1, and company 2 cells was found to be given, respectively, by:

$$E_t = E_{20^\circ C} - [40.44(t - 20) + 0.921(t - 20)^2 - 0.00866(t - 20)^3] \times 10^{-6} \text{ V},$$

$$E_t = E_{20^\circ C} - [40.14(t - 20) + 0.888(t - 20)^2 - 0.00668(t - 20)^3] \times 10^{-6} \text{ V},$$

$$E_t = E_{20^\circ C} - [39.28(t - 20) + 0.986(t - 20)^2 - 0.00943(t - 20)^3] \times 10^{-6} \text{ V}.$$

Values for the entropy and heat-capacity changes for the cell reaction in "acid" standard cells are also given.

**Pulse radiolysis of neopentane in the gas phase, R. E. Rebbert and P. Ausloos, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 4, 329-336 (July-Aug. 1972).**

**Key words:** Electron scavengers; gas phase; ion-molecule reactions; neopentane; neutralization; pulse radiolysis.

The pulse radiolysis of gaseous neopentane has been investigated in the absence and presence of electron scavengers ( $SF_6$ ,  $CD_3I$ ,  $CCl_4$ ). Deuterium labeling experiments show that the stable product molecules can be accounted for by (a) radical combination reactions involving mainly  $CH_3$  and  $H$ ; (b) hydride ion transfer reactions involving  $C_2H_5^+$ ,  $C_2H_5^+$ , and  $C_3H_5^+$ ; (c) neutralization reactions of  $C_4H_9^+$  and  $C_5H_{11}^+$ ; and (d) unimolecular dissociation of the parent ion ( $C_5H_{12}^+$ ) and of electronically excited neopentane. Neutralization of the  $t-C_4H_9^+$  ion, which is the major positive ion in the system, occurs as follows: (a)  $t-C_4H_9^+ + e \rightarrow i-C_4H_8 + H$  and (b)  $t-C_4H_9^+ + e \rightarrow 2CH_3 + C_3H_6$ . It is shown that  $C_5H_{11}^+$  produced in hydride ion transfer reaction  $C_nH_m^+ + \text{neo-}C_5H_{12} \rightarrow C_nH_{m+1} + C_5H_{11}^+$  (where  $C_nH_m^+ = C_2H_3^+$ ,  $C_2H_5^+$ , and  $C_3H_5^+$ ) rearranges to the  $CH_3C^+(CH_3)CH_2CH_3$  structure prior to neutralization. A detailed accounting of all products produced in the unimolecular and bimolecular reactions led to the conclusion that the ratio of neutral electronically excited molecules to parent ions ( $N_{ex}/N_+$ ) is 0.28.

**Anatomy and thermal history of laser self-focusing damage tracks in glass, W. Haller and J. H. Simmons, *J. Res. Nat. Bur. Stand. (U.S.)*, 76A (Phys. and Chem.), No. 4, 337-345 (July-Aug. 1972).**

**Key words:** Glass; laser damage; self-focusing.

Laser induced self-focusing damage tracks in glass are analyzed. The damaged regions consist of long cylinders of altered refractive index, containing occasional bubbles and partly surrounded by arrays of small cracks. An analysis of the refractive index change in the subfracture damage tracks and the presence of bubbles leads to estimates of a minimum temperature reached by heating of the glass in the tracks. A calculation of minimum stresses developed during laser-beam heating gives a good account of the orientation of the observed cracks.

**Normal emissivity of an isothermal, diffusely reflecting cylindrical cavity (with top) as a function of inside radius, W. B. Fussell, *J. Res. Nat. Bur. Stand. (U.S.), 76A (Phys. and Chem.), No. 4, 347-349 (July-Aug. 1972).***

**Key words:** Cavity; cylindrical cavity; diffusely reflecting; emissivity; normal emissivity; radiation; reflectance.

The normal emissivity of an isothermal cylindrical cavity (with top), with a diffusely reflecting interior of reflectivity much less than 1, is calculated approximately as a function of the inside radius of the cylinder by the DeVos method. The calculation is analytical, and considers the singly and doubly reflected radiation escaping from the cavity aperture. The results of the analysis indicate that, for cylinders whose length-to-lid aperture ratio is much larger than 1: (a), for a given cylinder length and lid aperture, the configuration with the inside diameter approximately 0.64 the length has the *smallest* normal emissivity; (b), as the inside diameter increases or decreases from the configuration of smallest normal emissivity, the normal emissivity *increases* monotonically.

**Lattice vibrations of antiparallel chain sheet structures, B. M. Fanconi, *J. Res. Nat. Bur. Stand. (U.S.), 76A (Phys. and Chem.), No. 4, 351-359 (July-Aug. 1972).***

**Key words:** Antiparallel chain sheet structures; honeycomb lattice; lattice vibrations.

Methods are developed for calculating the normal coordinate vibrations of isolated helical homopolymers and of the antiparallel sheet structures formed by some helical polymers in the solid state. The dynamical equations are expressed in Cartesian displacement coordinates starting from an internal coordinate harmonic force field. As an example of the method, the dynamical equations of the honeycomb lattice are derived.

## September-October 1972

**High accuracy spectrophotometry at the National Physical Laboratory, F. J. J. Clarke, *J. Res. Nat. Bur. Stand. (U.S.), 76A (Phys. and Chem.), No. 5, 375-403 (Sept.-Oct. 1972).***

**Key words:** High accuracy spectrophotometry; photoelectric linearity; reflectance; transmittance.

The techniques and equipment used at the National Physical Laboratory (NPL) to achieve high accuracy spectrophotometric measurements are described and discussed. The emphasis at NPL has always been on the determination of systematic components of error and their elimination or correction rather than on the attainment of mere precision, which is largely a matter of variance and resolution. The scales of regular transmittance, diffuse transmittance, total transmittance of scattering samples, regular reflectance, diffuse reflectance, total reflectance and radiance factor are determined, maintained, and made available in practical form to industry by combined use of a reference NPL manual spectrophotometer and commercial recording spectrophotometers.

The presentation will concentrate on transmittance measurements made with the reference instrument, which is designed specifically to allow separate investigation of the various possible sources of systematic error, processes that are not practicable with commercial spectrophotometers. The investigation of the linearity of the complete photoelectronic system has always been a key factor, and double-aperture devices have been used consistently at NPL for over 40 years to monitor the performance of this instrument and its predecessors. Besides instrumentation, the procurement of material standards of suitable quality is a major limitation of the art, and the types in use at NPL are described, including the recently developed Ceramic Colour Standards.

**An accurate spectrophotometer for measuring the transmittance of solid and liquid materials, R. Mavrodineanu, *J. Res. Nat. Bur. Stand. (U.S.), 76A (Phys. and Chem.), No. 5, 405-425 (Sept.-Oct. 1972).***

**Key words:** Absorbance; automation of accurate spectrophotometer; instrumentation, spectrophotometric; spectrophotometry, high accuracy; standard reference material in spectrophotometry; transmittance.

The optical transmittance of solids and liquids as well as the molar absorptivity of various chemical species are parameters of fundamental significance in characterizing these materials. Meaningful transmittance data can be obtained only when the measurements are performed with well-known accuracy and precision. To perform such measurements, a high accuracy spectrophotometer was designed and assembled at NBS, Analytical Chemistry Division, and will be described in this paper. This single-beam instrument is composed of a constant radiation source, a monochromator, a sample carriage, an integrating sphere-photomultiplier assembly followed by appropriate electronics, and a read out system consisting of a digital voltmeter and a computer data acquisition and handling provision. The accuracy of transmittance measurements is determined by the light-addition principle used in conjunction with a two-aperture arrangement. The spectrophotometer can be used in manual or automatic modes of operation. A detailed discussion of the data obtained with this instrument, used in both modes, will be presented together with its application to the certification of solid and liquid Standard Reference Materials for checking the photometric scales of conventional spectrophotometers.

**Absolute spectroradiometric measurements, G. A. W. Rutgers, *J. Res. Nat. Bur. Stand. (U.S.), 76A (Phys. and Chem.), No. 5, 427-436 (Sept.-Oct. 1972).***

**Key words:** Absolute spectroradiometry; absolute standard source of radiation; calibrated photodetector.

There are two general methods for measuring a quantity of radiation emitted by a source. One can compare it with the radiation emitted by a standard source or one can measure the radiation with a detector calibrated in absolute units. When using the latter method, one must know the spectral transmittance factor of the optical components between source and detector.

In the present paper, a survey will be given of the standard sources available for spectroradiometry: cavity radiator, tungsten strip lamp, anode of the carbon arc, xenon arc and cascade arc. Several types of detectors such as the absolute bolometer and thermopile, with their properties, will be discussed.

**Accurate measurements of and corrections for nonlinearities in radiometers, C. L. Sanders, *J. Res. Nat. Bur. Stand. (U.S.), 76A (Phys. and Chem.), No. 5, 437-453 (Sept.-Oct. 1972).***

**Key words:** Nonlinearity; photocell linearity; photometric accuracy; radiation addition method.



The methods described in the literature for accurately measuring photocell linearity are surveyed and assessed. The effects of not measuring photocell linearity under the conditions used in the final apparatus are considered. Some of the conditions necessary for accurate assessment of the nonlinearity under working conditions are specified. The use of the NRC "Photocell Linearity Tester" to measure and correct for the nonlinearity of various receivers is described.

**Physical parameters in high-accuracy spectrophotometry**, K. D. Mielenz, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 5, 455-467 (Sept.-Oct. 1972).

**Key words:** High accuracy spectrophotometry, physical parameters; linearity test of photodetector; spectrophotometry, high accuracy.

The measured apparent transmittance  $T_A$  of a filter or liquid sample depends on the beam geometry in the spectrophotometer. For focused light incident upon the sample,  $T_A$  is different for systems having different f-numbers, and also depends on the state of polarization of the light. These effects are eliminated when the incident light is collimated; in this case  $T_A$  approaches the "true" transmittance  $T$  of the sample. Both modes of operation suffer from stray light and interference effects. The former may be reduced significantly by using mirror rather than lens optics, and the latter by suitable choice of the monochromator slit width. A new spectrophotometer based upon the above-mentioned design principles is described. The photometric precision of this instrument is shot-noise limited, permitting measurements to better than  $10^{-4}$  transmittance units.

The double-aperture method of testing detector linearity to this level of precision is discussed. The conventional method of finding the nonlinearity correction can be replaced by a curve-fitting procedure giving better precision. Data on detector nonlinearity, and its dependence on wavelength, are presented.

**Liquid absorbance standards**, R. W. Burke, E. R. Deardorff, and O. Menis, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 5, 469-482 (Sept.-Oct. 1972).

**Key words:** Absorptivity data; liquid absorbance standards; Standard Reference Materials.

Errors in the measurement of the absorbances of liquid filters result from instrumental and chemical uncertainties. This paper presents a systematic study of these variables on the absorbances of selected filters. Three types of liquid filters are discussed. These are (1) individual solutions of high purity compounds, (2) composite mixtures, and (3) aqueous solutions of organic dyes. The accuracy of the absorptivity data is established using NBS-calibrated glass filters. The magnitude of the errors arising from spectral bandpass, beam geometry, stray light, internal multiple reflections, and refractive index are delineated. Finally, as a practical outgrowth of this study, the development and issuance of NBS Standard Reference Material 931, Liquid Absorbance Standards for Ultraviolet and Visible Spectrophotometry, is described.

**Accurate measurement of molar absorptivities**, R. W. Burnett, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 5, 483-489 (Sept.-Oct. 1972).

**Key words:** Molar absorptivity in clinical chemistry; random errors in molar absorptivity; systematic errors in molar absorptivity.

The key to accurate measurement of molar absorptivities is a thorough understanding of the sources of error which appear throughout the measurement procedure. Sources of determinant error will be listed with comments on estimating their magnitude and eliminating them where possible. Sources of random error

will be discussed as well as the propagation of both random and determinant errors. There is discussion of the need for accurate values of molar absorptivities using examples from clinical chemistry. Finally, the proper use of accurate absorptivity values in the clinical chemistry laboratory will be considered. Here, emphasis is on the need for a quality assurance system which includes routine checks on such things as wavelength calibration and photometric accuracy of spectrophotometers, calibration of analytical balances, and quality of incoming reagents.

**Problems associated with the need for standardization in clinical spectrophotometric and fluorometric measurements**, J. R. Panton, G. M. Widdowson, and G. Z. Williams, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 5, 491-498 (Sept.-Oct. 1972).

**Key words:** Clinical standards; standardization, spectrofluorometric; standardization, spectrophotometric; standard reference materials.

There is a growing demand in clinical chemistry for analyses to be performed in a manner allowing comparisons of results among laboratories and, from time to time, in the same laboratory. Reliable comparability requires adequate procedures of standardization for spectrophotometric and fluorometric instruments and methods. Problems with chemical and instrumental standardization are discussed.

For assays where the substance to be measured is available in suitable form, primary chemical standardization is justifiably popular. Relatively unsophisticated instrumentation can be used to compare measurements of unknown samples with such standards. Because primary standards meeting all necessary criteria are not available for many assays of clinical significance, standardization must depend on precision and accuracy of the instrumentation used, and on accurately compiled values of chemical-optical properties for the materials of interest. The task of compilation is outside the capability of the routine laboratory and should be provided by a reliable central agency. If an individual laboratory is to use the agency's compiled values, that laboratory must have available precise, accurate and reasonably inexpensive instrumentation along with reliable absorbance, fluorescence, and wavelength calibration standards.

**The role of spectrophotometric standards in the clinical chemistry laboratory**, R. N. Rand, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 5, 499-508 (Sept.-Oct. 1972).

**Key words:** Clinical spectrophotometry, accuracy, precision; optical cuvettes; spectrophotometric standards, clinical.

It is obvious that erroneous data reported to a physician may adversely affect patient welfare. Currently, acceptable limits of accuracy and precision are poorly defined. It should be recognized, however, that the spectrophotometric measurement step in an appropriate analytical procedure is critical and inapparent error may occur. Spectrophotometric measurements, both manual and automated, are extensively used in the clinical chemistry laboratory. At least 1,000,000 such measurements per day on rather diverse equipment are made in this country; yet, few standards exist. Results of intra-lab surveys suggest that performance could be improved. The various ways in which spectrophotometry is used will be illustrated and a discussion of possible errors resulting from nonstandardized instrumentation will follow. There is pressing need for well defined and easily usable standards for wavelength, photometric accuracy, photometric linearity, stray light, as well as NBS specifications for optical cuvettes.



**Spectrophotometric standards**, W. H. Venable, Jr., *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 5, 509-510 (Sept.-Oct. 1972).

**Key words:** Photometric accuracy; standards, spectrophotometric.

To be useful, spectrophotometric measurements must be believable and practical. The basic standard for any believable spectrophotometric measurements is the ability to accurately compare fluxes of radiation within the framework of a well-defined geometry. The emphasis in the program proposed for the Institute for Basic Standards is to develop such ability over the broadest range of spectrophotometric measurements. Establishing such a basis will enable the National Bureau of Standards to render real assistance to those who deal with the problem of making practical measurements.

**An alternative to accurate pyrometry in distinguishing concurrent vaporization reactions. Postulated results using the vaporization of gold in analyzing the vaporization of beryllium oxide in water vapor**, T. B. Douglas, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 5, 511-515 (Sept.-Oct. 1972).

**Key words:** Beryllia hydrates (gases); contaminants; gold; pyrometry; reference vaporization; temperature consistency; thermodynamic parameters (estimated).

For the transpiration determination of vaporization properties whose interconsistency is critical, the simultaneous vaporization of a reference substance such as uncontaminated gold is suggested as an alternative to accurate pyrometry. Calculations suggest that gold would be superior to all but the most accurate pyrometry in the temperature range 1700 to 2300 K. An application to seeking unreported gaseous hydrates of beryllia is illustrated by calculations based on estimated thermodynamic parameters.

**The determination of iron, titanium, and nickel in Apollo 14 samples by cathode ray polarography**, E. J. Maienthal, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 5, 517-520 (Sept.-Oct. 1972).

**Key words:** Analyses of iron, titanium, nickel; Apollo 14 lunar samples; differential cathode ray polarography.

Methods have been developed and applied to the determination of iron, titanium, and nickel in Apollo 14 fine soil and rock by differential cathode ray polarography on the same sample. A 5 mg sample was sufficient for the determination of all 3 elements. Iron and titanium were determined either directly or after cupferron separation. Nickel was determined after dimethylglyoxime separation.

**The Stark splitting of millimeter wave transitions of water**, Y. Beers and G. P. Klein, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 5, 521-528 (Sept.-Oct. 1972).

**Key words:** Millimeter waves; Stark effect; water.

This paper first discusses the technique of making Stark measurements at millimeter wavelengths. The details of correcting for residual overlap between the lines, the effects of modulation, and of the field inhomogeneity are discussed. Finally the measured frequencies and the empirical Stark coefficients for one H<sub>2</sub>O and one D<sub>2</sub>O and five HDO lines between 85 and 250 GHz are given. The final analysis of the data to give values of the dipole moment will be given in another paper.

## November-December 1972

**Absolute spectrofluorometry**, W. H. Melhuish, *J. Res. Nat. Bur.*

*Stand. (U.S.)*, **76A**, (Phys. and Chem.), No. 6, 547-560 (Nov.-Dec. 1972).

**Key words:** Actinometers; calibration of spectrofluorometers; detectors, absolute; fluorescence spectra, corrected; quantum counters; spectrofluorometers, design; spectrofluorometry, absolute; standard lamps; standards, fluorescence; thermopiles.

The last 10 years has seen the increasing publication of the emission spectra of organic, inorganic and metal-chelate compounds, but there is no agreed method of presentation of such spectra. In the few cases where corrected emission spectra have been published, there is often no mention of the units used for the intensity coordinate or the method used for correcting spectra. A method of reporting absolute fluorescence spectra originally put forward in 1962 will be reexamined and improved. The two best known methods for calibrating spectrometers for absolute spectrofluorometry: (a) standard tungsten lamp, (b) quantum counter method, will be critically examined, and the limitations and possible improvements in accuracy will be proposed. The criteria for an emission standard will be examined and the use of emission standards for calibrating spectrofluorometers discussed. It is suggested that the distribution of emission standards to laboratories measuring corrected fluorescence spectra and the analysis and publication of the results should be done in the near future.

**Absolute quantum efficiencies**, G. A. Crosby, J. N. Demas, and J. B. Callis, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 561-577 (Nov.-Dec. 1972).

**Key words:** Calorimetry in quantum yields; laser, use in quantum yields; photodetectors in quantum yields; quantum efficiencies.

Recent developments in several areas of chemistry, laser technology, photodetector instrumentation, and calorimetry are surveyed, and their probable impact on the measurement of quantum yields is assessed. Chemical developments include: (a) synthesis and design of new luminescent molecules that could possibly serve as standards, (b) application of improved separation techniques to provide samples of extreme purity, and (c) advances in photochemistry that portend the development of wide-range chemical actinometers. The potential use of lasers in quantum yield measurements and their advantages over conventional sources for application in both optical and calorimetric techniques are pointed out. New methods of quantum yield measurements, based on the novel characteristics of laser pump sources, are suggested, including the feasibility of measuring yields under time-resolved conditions and of employing internal standards. The possible lifting of wavelength restrictions on both laser sources and detector devices and the implications of these developments for extending the spectral range of quantum yield measurements are discussed. The current status of calorimetry for determining yields is surveyed, and the impact of recent technology on the feasibility of developing calorimetric methods competitive with optical methods is assessed.

**Phosphorimetry**, J. D. Winefordner, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 579-592 (Nov.-Dec. 1972).

**Key words:** Aqueous solvents in phosphorimetry; phosphorimetry; rotating capillary cell; solvents for phosphorimetry.

Phosphorimetry in the past has received limited use because the precision of reproducibility was inadequate, there were solvent limitations, and preparation of test specimens was difficult and time consuming. Detection limits have now been lowered by more than two orders of magnitude by using a rotating capillary

sample cell, a more stable excitation-source power supply, and aqueous solvents. These steps have also increased precision by more than an order of magnitude. Considerable reduction in time and effort of sampling and measurements has been effected compared to phosphorimetric measurements made with standard procedures and commercial equipment. Twenty microliters of aqueous solution is all that is required to fill a quartz capillary cell by capillary action. Capillary cells filled with aqueous solutions do not crack when cooled to 77 K or when returned to room temperature. Rotation of the sample cell minimizes effects due to cell orientation and thus improves precision. Reduction of background phosphorescence results in improved accuracy of analysis. A study was made of the influence of methanol-water mixtures and of sodium-halide aqueous solutions on the magnitude of phosphorescence signals from several substances and of the effect on signal-to-noise ratios. The optimum solvent system for many phosphorimetric measurements is discussed. Analytical results are given for several organic substances measured by phosphorimetry at 77 K. These results are compared with those from previous studies by older methods.

**Measurements of absolute values in biochemical fluorescence spectroscopy**, R. F. Chen, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 593-606 (Nov.-Dec. 1972).

**Key words:** Absolute fluorometry; absolute fluorometry in biochemistry; standard reference materials in fluorometry.

Fluorescence spectroscopy is an important tool of the biochemist studying the structure and interactions of proteins and nucleic acids. The four basic quantities to measure accurately are: (1) spectra (corrected excitation and emission), (2) quantum yields ( $Q$ ), (3) fluorescence decay characteristics, and (4) polarization. Commercially available instruments, with little modification, can be used to obtain these measurements, but the biochemist in this field is very dependent on the accuracy of measurements of substances he uses as standards. Confusion arises from disagreement between reported values for standards which may be used to calibrate a detector system to obtain quantum yields, or to set up lifetime and polarization photometers. For instance, the protein chemist is fond of using tryptophan and quinine as quantum yield standards, but  $Q$  for tryptophan has been variously reported as 0.13 and 0.20, and  $Q$  values for quinine bisulfate range from 0.4 to 0.7. The biochemist should also be aware of the problems inherent in the use of commercially available instruments in absolute measurements, as well as the special complications arising in complex biochemical systems where the fluorescence is heterogeneous.

**Newer fluorometric methods for the analysis of biologically important compounds**, G. G. Guilbault, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 607-612 (Nov.-Dec. 1972).

**Key words:** Enzymes, fluorometric analysis; fluorometry of enzymes; fluorometry of substrates; silicone pad; solid surface fluorometry.

Newer fluorometric methods for the analysis of biologically important compounds will be discussed: enzymes such as LDH, alkaline phosphatase, lipase and cholinesterase, and substrates such as glucose, urea and uric acid. These methods are based on the production of fluorescence initiated by an enzymic reaction.

New reagentless fluorescence methods will be described for enzymes and substrates. These methods are highly precise (1%), fast (less than 1 minute) and involve no preparation of reagents. These methods, as adapted to clinical laboratory procedures, will be discussed.

**Inorganic ions in glasses and polycrystalline pellets as fluorescence standard reference materials**, R. Reisfeld, *J. Res. Nat. Bur.*

*Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 613-635 (Nov.-Dec. 1972).

**Key words:** Fluorescence standards, inorganic ions; glass standards in fluorescence; rare-earth-doped glasses.

The absorption and fluorescence of inorganic glasses and polycrystalline disks doped by heavy metal ions is discussed, and their use as fluorescence standards is evaluated. The advantages of the glass standards over other media are summarized.

The glass standards are divided into two groups: (1) glasses doped by trivalent rare earths such as  $Gd^{3+}$ ,  $Tb^{3+}$ ,  $Eu^{3+}$ ,  $Sm^{3+}$ , and  $Tm^{3+}$  which have narrow band optical spectra as a result of intraconfigurational transitions, and (2) glasses and polycrystalline disks doped by ions such as  $Tl^{+}$ ,  $Pb^{2+}$ ,  $Ce^{3+}$ , and  $Cu^{+}$  which have broad spectral bands since the optical spectra originate from interconfigurationally allowed transitions. Optical and physical parameters, including matrix effects, quantum efficiencies, decay characteristics, Stokes' shifts and spin-orbit versus orbit-lattice interactions due to the different transitions will be discussed.

Group (1) glasses are suitable for use as standards where a narrow well-defined fluorescence range is required, and group (2) glasses are suitable for use as standards whenever a substance with a wide range of fluorescence is measured. Special emphasis will be placed on energy transfer between donor and acceptor ions.

**Development of a new fluorescent reagent and its application to the automated assay of amino acids and peptides at the picomole level**, S. Udenfriend, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 637-640 (Nov.-Dec. 1972).

**Key words:** Fluorometry, amino acids; fluorometry, peptides; picomole fluorometry.

Methods for the assay of amino acids and peptides are most important in elucidating the structure of proteins and peptides. In many important areas of research such as in endocrinology, neurobiology, and genetics, methods are needed with sensitivity higher than is available with the widely used colorimetric ninhydrin procedure. A short while ago, we noted that all primary amines react with ninhydrin and phenylacetaldehyde to give a ternary product which is highly fluorescent. The chemistry of that reaction has now been elucidated and the conditions have been modified and improved so that essentially quantitative yields of fluorescent products are formed with all primary amines. The reaction has been automated and is being used as the detecting system for chromatography of amino acids, peptides and amines in the 10 to 100 picomole range. Problems concerning the fluorescence instrumentation and the isolation and chromatography of these compounds in the picomole range will be discussed.

**Considerations on organic compounds in solution and inorganic ions in glasses as fluorescent standard reference materials**, R. A. Velapoldi, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 641-654 (Nov.-Dec. 1972).

**Key words:** Emission spectra; excitation spectra; fluorescence; fluorescence standards; glass standards; quinine derivatives; rare earths; relative quantum efficiencies; solution standards.

The use of various organic compounds in solution and inorganic ions in glasses has been investigated as possible fluorescence Standard Reference Materials. Emphasis was placed on measuring physical and chemical parameters such as stability, reproducibilities of absorbance and fluorescence measurements, relative quantum efficiencies as a function of excitation wavelength, etc., for quinine derivatives and selected or-

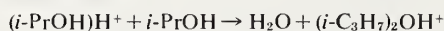


ganic compounds. A brief discussion is included on the use of rare earth and non-rare earth inorganic ions in glasses as standards.

**Ion-molecule reactions in isopropanol: Implications for its radiolysis,** R. Gorden, Jr., and L. W. Sieck, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 655-659 (Nov.-Dec. 1972).

Key words: Gas-phase kinetics; ion-molecule reactions; mass spectrometry; photoionization; proton affinity; radiolysis.

The photoionization of isopropanol (*i*-PrOH) at 11.7 eV has been investigated in the NBS high pressure photoionization mass spectrometer over the pressure range 0.1 to approximately 200 millitorr. The major primary ion,  $\text{CH}_3\text{CHOH}^+$ , reacts with a total rate coefficient of  $1.1 \pm 0.1 \times 10^{-9} \text{ cm}^3/\text{molecule} \cdot \text{s}$  to yield mainly (*i*-PrOH) $\text{H}^+$  and  $\text{CH}_3(i\text{-C}_3\text{H}_7)\text{COH}^+$ . At pressures in excess of a few millitorr consecutive reactions of (*i*-PrOH) $\text{H}^+$  and  $\text{CH}_3(i\text{-C}_3\text{H}_7)\text{COH}^+$  were also detected, including the overall dehydration process



These data are interpreted in light of a recent radiolysis study, and a thermal cationic chain mechanism for production of (*i*-C<sub>3</sub>H<sub>7</sub>)<sub>2</sub>O consistent with those results is proposed. The value for the proton affinity of SF<sub>6</sub> is also discussed in some detail.

**Excitation of  $\text{O}_2^1\Delta_g$  by electron impact,** P. S. Julienne and M. Krauss, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 661-663 (Nov.-Dec. 1972).

Key words: Ab initio Gaussian wave functions; electron impact excitation; exchange amplitude;  $\text{O}_2^1\Delta_g$  state; Ochkur-Rudge approximation.

The total and differential cross sections as a function of energy were calculated for electron impact excitation of the  $\text{O}_2^1\Delta_g$  state for the ground  $^3\Sigma_g^-$  state. The Ochkur-Rudge approximation was used for the exchange amplitude, which was calculated using Hartree-Fock wave functions with a Gaussian basis; there is good agreement with the experimental total cross section except near threshold.

**Vibrational and electronic oscillator strengths of LiO,** M. Marchetti, P. S. Julienne, and M. Krauss, *J. Res. Nat. Bur. Stand. (U.S.)*, **76A** (Phys. and Chem.), No. 6, 665-668 (Nov.-Dec. 1972)

Key words:  $A^2\Sigma$ ; electronic transition probabilities; Hartree-Fock; LiO; vibrational transition probabilities;  $X^2\Pi$ .

Electronic energies and wave functions of ground and excited states of LiO are calculated in the Hartree-Fock approximation. The vibrational oscillator strengths of the  $X^2\Pi$  and  $A^2\Sigma^+$  valence states are calculated for  $v=0$  to 1 and 1 to 2 transitions. Electronic oscillator strengths are also presented for transitions to the quantum number of two Li Rydbergs. Reasons are presented to support the use of the Hartree-Fock approximation.



## 3.2. PAPERS FROM THE JOURNAL OF RESEARCH OF THE NATIONAL BUREAU OF STANDARDS, SECTION B. MATHEMATICAL SCIENCES, VOLUME 76B, JANUARY-DECEMBER 1972

### January-June 1972

**Minimax-based selection, adjustment and disaggregation for incompletely specified univariate distributions**, A. J. Goldman, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 1 and 2, 1-38 (Jan.-June 1972).

Key words: Linear programs; mathematical models; minimax estimation; operations research; probability distribution.

This paper deals with making a nominal choice from a class of discrete univariate probability distributions about which one has "incomplete information" such as component-wise bounds, a component-wise ranking, or both. In some cases, an initial distribution is provided, to be "adjusted" so as to be compatible with the incomplete information. The first part of the analysis systematizes and unifies the contents of four earlier papers treating such problems using a minimax-error or minimax-adjustment approach. The second part applies the same approach to situations in which an "aggregate" of the desired distribution is stipulated, either exactly, or approximately by component-wise bounds. All problems discussed in the paper can be formulated as linear programs, but relatively explicit solution methods are sought; unresolved difficulties arising in this attempt are identified.

**Three results for trees, using mathematical induction**, W. A. Horn, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 1 and 2, 39-43 (Jan.-June 1972).

Key words: Helly's theorem; mathematical induction; minimum-length coverings; node-covering; trees.

The paper illustrates the use of mathematical induction to extend results which are true for a line segment to trees. Three separate theorems are stated and proved, each of which has some importance in its own right.

**Abstract groups as doubly transitive permutation groups**, R. Merris, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 1 and 2, 45-50 (Jan.-June 1972).

Key words: Character; cosets; matrix representation; nilpotent group; normalizer; solvable group.

The question considered is this: Which abstract groups have representations as doubly transitive permutation groups? Moreover, given an abstract group, can all doubly transitive representations be found? The paper is expository. Various results which bear on the question are presented in an elementary way.

**Covariances of two sample rank sum statistics**, P. V. Tryon, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 1 and 2, 51-52 (Jan.-June 1972).

Key words:  $c$  Sample problem; covariances; Mann-Whitney-Wilcoxon statistics; rank sum statistics; statistics.

This note presents an elementary derivation of the covariances of the  $c(c-1)/2$  two-sample rank sum statistics computed among all pairs of samples from  $c$  populations.

**Efficient techniques for unbiasing a Bernoulli generator**, J. A. Lechner, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 1 and 2, 53-60 (Jan.-June 1972).

Key words: Bernoulli; binomial; coin-tossing; computer; efficiency; generator; random numbers; statistics.

Consider the problem of operating on a sequence of i.i.d. Bernoulli variables with unknown mean  $p$  to produce a sequence of symmetric Bernoulli variables. Define the efficiency of any proposed method to be the average number of binary output digits per input digit. The following results are proved: (A) No method exists having efficiency greater than  $-\log_2 p - q \log_2 q$ , where  $q = 1 - p$ . (B) Methods do exist with efficiency arbitrarily close to the bound just given. Examples are given, and compared with other methods in the literature. A technique for finding the methods of (B) above is given.

**Checks of the algebraic matrices for the configurations  $(d+s)^n p$** , C. Roth, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 1 and 2, 61-80 (Jan.-June 1972).

Key words: Checking parameters;  $(d+s)^n p$ ; electrostatic interaction; relative phases; spin-orbit interaction.

By constructing suitable combinations of algebraic matrices enabling the resulting eigenvalues to be predicted theoretically, checking parameters were obtained for 32 interaction parameters of the configuration  $(d+s)^n p$ .

### July-December 1972

**"Plural-series" approximations of functions**, L. V. Spencer, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 91-108 (July-Dec. 1972).

Key words: Biorthogonal function; gamma-ray transport; moment methods; neutron transport; polynomial representations; radiation penetration.

A method is given for developing approximations to neutron and gamma-ray transport distributions in the form of a superposition of  $U_n^k$  polynomial series multiplied by exponentials and characterized by different scale factors. Convergence conditions and error bound expressions are given. Biorthogonality properties are worked out. Examples are given in which these approximations are compared with polynomial approximations.

**Scheduling a time-shared server to minimize aggregate delay**, A. J. Goldman, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 109-117 (July-Dec. 1972).

Key words: Computer systems; optimization; scheduling; time-sharing.

A simplified analysis is given of a problem situation, previously treated in the literature, which pertains to the delay-minimizing allocation of servicing times among  $N$  incoming streams requiring "processing" of some kind by a single "server" (e.g., a time-shared computer). The original problem is generalized to permit different "weights" for the delays suffered by different streams.

**Normal matrices with entries from an arbitrary field of character  $\neq 2$ ,** M. H. Pearl and A. I. Penn, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 119-143 (July-Dec. 1972).

**Key words:** Field; matrices; normality.

Let  $F$  be an arbitrary field of characteristic  $\neq 2$  and let conjugation in  $F$  be defined by an arbitrary involutory automorphism (possibly the identity mapping). A matrix with entries from  $F$  is normal if it commutes with its conjugate transpose. Several conditions which are equivalent to normality when  $F$  is the complex field are properly nested when  $F$  is an arbitrary field. Of these conditions, normality is the weakest and unitary diagonalizability is the strongest.

When the underlying field is closed the unitarily diagonalizable matrices are those which possess a spectral representation with Hermitian idempotents. These matrices may be characterized in terms of their  $EP$  properties.

A matrix is indecomposable if it has a single elementary divisor of the form  $(x-s)^1$ . For  $i > 1$ , normal indecomposable matrices do not exist when  $F$  is the complex field. However there exists field for which normal indecomposable matrices of all finite orders exist. A matrix is a normal indecomposable matrix if and only if it can be expressed as  $r(B)$  where  $r(x)$  is a polynomial such that  $r(0) \neq 0$  and  $B$  is a matrix having the single elementary divisor  $x^i$  and satisfying the equation  $B^* = sB$  for some scalar  $s$ .

When the involutory automorphism of  $F$  is the identity mapping indecomposable normal matrices of even order exist if and only if the vector space  $F^n$  is hyperbolic, and in this case the matrices are symmetric. Moreover, indecomposable normal matrices of odd order exist if and only if  $F^n$  is the orthogonal sum of a hyperbolic space and a one dimensional space, and in this case both symmetric and nonsymmetric indecomposable normal matrices exist.

**Distance coordinates with respect to a triangle of reference,** K. Goldberg, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 145-152 (July-Dec. 1972).

**Key words:** Area coordinates; distance coordinates; Plane Geometry; radical center; triangle of reference.

With respect to a triangle of reference  $A_1A_2A_3$ , each point  $P$  in the plane of the triangle, has unique area coordinates:  $P = (b_1, b_2, b_3)$  with  $b_1 + b_2 + b_3 = 1$ . Distance coordinates are introduced such that  $P = [d_1, d_2, d_3]$ , with  $d_k$  the distance from  $P$  to  $A_k$ . It is shown that there is an explicit function  $f(x_1, x_2, x_3)$  such that  $f(d_1^2, d_2^2, d_3^2) = 0$  is necessary and sufficient for  $P = [d_1, d_2, d_3]$ , each  $d_k$  nonnegative. The partial derivatives  $f_k(x_1, x_2, x_3) = \partial f(x_1, x_2, x_3) / \partial x_k$  are such that  $b_k = f_k(d_1^2, d_2^2, d_3^2)$  for each  $k$ . Other results relating the  $b_k$  and the  $d_k$  are given. The use of  $f(x_1, x_2, x_3)$  in solving geometric problems is shown.

**On regular sets of polynomials whose zeros lie in prescribed domains,** M. A. Farag and M. Nassif, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 153-159 (July-Dec. 1972).

**Key words:** Basic sets; Cannon sum of basic sets; lower semiblock matrices; order of basic sets; zeros of polynomials in regular sets.

The relation between the mode of increase of regular basic sets of finite span and the order of magnitude of the zeros of polynomials  $\{p_n(z)\}$  belonging to them is investigated. Upper bounds are obtained for the order of the basic sets when the zeros of  $p_n(z)$  lie either in the unit circle or in a circle whose radius increases in a certain manner with the index  $n$  of the polynomial.

**The Stieltjes Constants,** J. J. Y. Liang and J. Todd, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 161-178 (July-Dec. 1972).

**Key words:** Bernoulli numbers; Euler-Maclaurin method; Euler transform; Euler's constant; multiple precision package; Riemann zeta function.

The Stieltjes Constants are the coefficients in the Laurent expansion of the Riemann Zeta function  $\xi(z)$  about its simple pole at  $z = 1$ . They can be represented as the limit of the difference between the sum of the first  $n$  terms of a series and the integral of its  $n$ -th term.

The first 20 coefficients have been computed to 15  $D$  using the Euler-Maclaurin method. As a by-product the sums of the series

$$\tau_n = \sum_{k=2}^{\infty} (-1)^k (\log k)^n / k$$

have been obtained to 15  $D$  for  $n = 1(1)20$ .

**Confidence limits for the abscissa of intersection of two linear regressions,** J. J. Filliben and J. E. McKinney, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 179-192 (July-Dec. 1972).

**Key words:** Abscissa; confidence limits; glass transition; intercept; intersection; linear; regression; second order transition; statistics; variance.

A method to determine the confidence limits for the abscissa of the intersection of two linear regressions has been developed. This method does not require the assumption of equal variance for the two regressions, as was necessary with previous methods. A numerical example is included on thermodynamic, glass transition data for which this method is applicable. Comparisons are made between the results using equal and unequal variance assumptions. A FORTRAN subroutine is included for computations using both assumptions.

**Weighting methods for Monte Carlo calculation of polymer configurations,** F. L. McCrackin, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 193-200 (July-Dec. 1972).

**Key words:** Boltzmann factors; importance sampling; Monte Carlo; non-self-intersecting walks; polymer configurations; random walks.

In the Rosenbluth and Rosenbluth method of computing polymer configurations, the configurations are weighted in order to remove bias of the estimated parameters of the configurations. This weighting method is investigated and generalized for importance sampling and Boltzmann factors. The estimates are found to be unbiased in the limit for an infinite sample of configurations, but to have a bias for a finite sample. The standard deviations of the estimates are also derived.

**Product solutions and separation of variables,** A. J. Goldman, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 201-204 (July-Dec. 1972).

**Key words:** Difference equations; functional equations; separation of variables.

This paper consists of two independent notes, whose common features are (a) their concern with "product-form" functions and (b) their use of an abstract-algebra setting to isolate the essential features of the problems treated. The first note further generalizes the generalizations given by Chu and Diaz (1965) of their observation that Euler's difference equation  $y(x+1) - y(x) = f(x)$ , when  $f$  is of period 1, has the product-form solution

$y(x)=xf(x)$ . The second note formalizes and rigorously proves the fact that a function is separable jointly in its variables if it is separable in each individual variable.

**A note of the multiplicative property of the Smith normal form,**  
M. Marcus and E. E. Underwood, *J. Res. Nat. Bur. Stand. (U.S.)*, **76B** (Math. Sci.), Nos. 3 and 4, 205-206 (July-Dec. 1972).

Key words: Compound; divisors; matrix.

This paper contains an elementary proof of the fact that if  $A$  and  $B$  are  $n$ -square matrices over a principal ideal domain  $R$  with relatively prime determinants then  $S(AB)=S(A)S(B)$  where  $S(A)$  is the Smith normal form of  $A$ .



### 3.3. PAPERS FROM THE JOURNAL OF RESEARCH OF THE NATIONAL BUREAU OF STANDARDS, SECTION C. ENGINEERING AND INSTRUMENTATION, VOLUME 76C, JANUARY-DECEMBER 1972

Effective with this issue, this Section was discontinued.

#### January-June 1972

**National Bureau of Standards one kilogram balance (NBS No. 2),** H. E. Almer, *J. Res. Nat. Bur. Stand. (U.S.), 76C* (Eng. and Instr.), Nos. 1 and 2, 1-10 (Jan.-June 1972).

Key words: Arrestment; balance; beam; buoyant; case; constant-load; equilibrium; knife; one-pan; short arm; two-knife.

The balance described is a one-pan, two-knife, short arm, 1 kg balance. The fulcrum flat and the suspension support elements are mounted on a bed plate supported by three posts attached to the base. The weight handling mechanism is mounted on a center column attached to the base. The balance has two modes of arrestment, the constant load mode and the full arrest mode. A double case encloses the structure.

There are positions for six weights inside the balance. These weights can be compared with each other, according to an appropriate weighing design, without opening the balance case. The operation of the balance and the weight changing are through control elements outside the balance case. The indicating elements for the instruments measuring the pressure, temperature, and relative humidity within the balance are located inside the balance.

The standard deviation of the balance developed by a series of measurements in the National Bureau of Standards Experimental Mass Laboratory was approximately  $4\mu\text{g}$ .

**Ball and cylinder interferometer,** J. B. Saunders, Sr., *J. Res. Nat. Bur. Stand. (U.S.), 76C* (Eng. and Instr.), Nos. 1 and 2, 11-20 (Jan.-June 1972).

Key words: Density standards; interferometer; volume of spheres.

An interferometer is described that permits the comparison of diameters of balls and cylinders with an etalon. The specimen is located in the cavity of the etalon. Interference is produced by light reflected from each surface of the etalon and the adjacent surface of the specimen. The two pairs of interfering beams of light (one pair from each side of the etalon) are received by the same eyepiece or camera. A shutter permits alternate viewing of the two interferograms. Magnification and contrast of the fringes are obtained by a suitable choice of power and separations of components of the system. After the prime dimension of the etalon is determined, it can be subsequently rechecked with the single mode (stabilized) laser, used with this interferometer, without removing the etalon from the assembly. A method is provided for analyzing the results of this interferometer.

**Precision reference specimens of surface roughness: Some characteristics of the Cali-Block,** R. D. Young and F. E. Scire, *J. Res. Nat. Bur. Stand. (U.S.), 76C* (Eng. and Instr.), Nos. 1 and 2, 21-23 (Jan.-June 1972).

Key words: Arithmetic Average roughness; Cali-Block; calibration; roughness.

The distribution of Arithmetic Average values of surface roughness across the 120 and 20 micro-inch patches of NBS

Cali-Block "B" have been measured. It is shown that each distribution can be described in terms of its mean value and standard deviation. The observed systematic distribution of  $AA$  values strongly suggests that the user select several widely spaced regions at random on the patch when calibrating a roughness measuring instrument.

**Absorption of sound in liquids by the resonator-decay technique: A critique,** M. Greenspan, *J. Res. Nat. Bur. Stand. (U.S.), 76C* (Eng. and Instr.), Nos. 1 and 2, 25-32 (Jan.-June 1972).

Key words: Acoustic impedance; acoustic materials; acoustic parameters; acoustics.

(1) The resonator-decay and the reverberation methods for measurement of the absorption of sound in liquids are in wide use, but their theoretical foundation has not hitherto been investigated. The basic assumptions are in fact invalid, but under most practical conditions the errors are tolerable, at least for three common geometries. (2) The very large excess losses always observed at the lower-order modes are identified with anelastic effects in the envelope, for the most part, and with viscous boundary-layer effects to a lesser, but very substantial extent. For modes of sufficiently high order these become negligible.

**Ductile fracture by development of surfaces of unstable cavity expansion,** C. A. Berg, *J. Res. Nat. Bur. Stand. (U.S.), 76C* (Eng. and Instr.), Nos. 1 and 2, 33-39 (Jan.-June 1972).

Key words: Ductile fracture; plasticity; void growth.

A model of fracture of a ductile metal in which surfaces of unstable microcavity expansion occur is proposed. It is shown that such surfaces can occur only in locally plane incremental strain. The hardening conditions required for the development of these surfaces are considered. It is shown that in a material possessing an equivalent yield stress ( $Y$ ) which depends upon the total plastic dilatation ( $\Delta$ ) and equivalent distortional strain ( $\epsilon$ ), the minimum ratio of dilatational softening ( $\partial\gamma/\partial\Delta < 0$ ) to distortional hardening ( $\partial\gamma/\partial\epsilon > 0$ ) under which an unstable surface of a dilatation may form is  $-2/3$ . A possible explanation, based upon the model, for the lack of correlation between plane strain ductility and ductility as measured in a tensile test is offered. Also, the pertinence of the model to fracture of glassy polymers and environmental stress cracking of crystalline polymers is discussed.

**Friction and wear of graphite fiber composites,** C. A. Berg, S. Batra, and J. Tirosh, *J. Res. Nat. Bur. Stand. (U.S.), 76C* (Eng. and Instr.), Nos. 1 and 2, 41-52 (Jan.-June 1972).

Key words: Composites; friction; graphite fiber; wear.

Friction and wear of two different types of graphite fiber composites were studied in a pin-disk sliding contact wear machine. Composites reinforced (62% by volume) with low modulus, high strength circular fiber (Modmor II) exhibited very high resistance to wear [a threshold wear load of  $\sim 20$  N, a maximum bearing load of  $\sim 50$  N, and a wear coefficient of  $\sim 10^{-6}$ ] when worn by hardened steel pins. However, the composite produced extreme abrasion on the steel counterface. Composites rein-

forced (62% by volume) with high modulus, lower strength, non-circular fiber (GY70) also exhibited high resistance to wear (a threshold wear load of  $\sim 25$  N, a maximum bearing capacity of  $\sim 20$  N, and a wear coefficient of  $\sim 10^{-6}$ ) when worn by hardened steel, but these composites developed a surface film which prevented abrasional damage to the steel counterface.

Potential applications of the two different types of composites in bearings are discussed. The advantages of these composites in bearings subject to corrosion, vibration, loss of lubrication, or impact damage are noted.

**A note on construction of the equivalent plastic strain increment,**  
C. A. Berg, *J. Res. Nat. Bur. Stand. (U.S.)*, **76C** (Eng. and Instr.), Nos. 1 and 2, 53-54 (Jan.-June 1972).

Key words: Equivalent strain; hardening; plasticity; strain hardening; work hardening.

Strain hardening plastic deformation of a material possessing a yield locus which may be written as a homogeneous function of the stress components, and which obeys the classical associated flow rule for metals is considered. The material may be anisotropic and may display plastic dilatation. A method is given for constructing the equivalent plastic strain increment in such a way that the increment of plastic work is always equal to the product of the equivalent plastic strain increment and the equivalent yield stress. The method is implied in classical treatments of hardening but seems not to have been given explicitly heretofore.



### 3.4. MONOGRAPHS

Major contributions to the technical literature on various subjects related to the Bureau's scientific and technical activities.

Monogr. 25, Section 10. **Standard x-ray diffraction powder patterns. Section 10—Data for 84 substances**, H. E. Swanson, H. F. McMurdie, M. C. Morris, E. H. Evans, B. Paretzkin, J. H. deGroot, and S. J. Carmel, Nat. Bur. Stand. (U.S.), Monogr. 25, Sec. 10, 161 pages (Nov. 1972).

Key words: Crystal structure; integrated intensities; lattice constants; peak intensities; powder patterns; reference intensities; standard; x-ray diffraction.

Standard x-ray diffraction patterns are presented for 84 substances. Forty-seven of these patterns represent experimental data and 37 are calculated. The experimental x-ray powder diffraction patterns were obtained with an x-ray diffractometer. All d-values were assigned Miller indexes determined by comparison with computed interplanar spacings consistent with space group extinctions. The densities and lattice constants were calculated, and the refractive indexes were measured whenever possible. The calculated x-ray powder diffraction patterns were computed from published crystal structure data. Both peak height and integrated intensities are reported for the calculated patterns.

Monogr. 122. **Mechanics of pneumatic tires**, S. K. Clark, Editor, Nat. Bur. Stand. (U.S.), Monogr. 122, 853 pages (Nov. 1971).

Key words: Friction; rubber; skid; tire contact; tire cord; tires; tire stress; tire structure; vehicles.

The pneumatic tire has been an integral part of automotive transportation almost since its inception, yet it remains a product whose characteristics are not easily predictable or comprehensible by conventional engineering techniques. This treatise is an attempt to provide a rational descriptive and analytical basis for tire mechanics. Chapters of this book are contributed by active research workers in the fields of rubber and textile properties, friction, material properties, tire stress problems, tire design and construction, vehicle skid and handling, and tire mechanical properties.

Monogr. 123. **BOLOVAC systems for measuring electrical quantities from 0.5 MHz through microwaves**, M. C. Selby, Nat. Bur. Stand. (U.S.), Monogr. 123, 24 pages (Jan. 1972).

Key words: BOLOVAC; calibration of current meters through microwaves; calibration of power meters through microwaves; calibration of voltmeters through microwaves; current measurement; disk-type bolometer evaluation; frequency-domain pulse evaluation; measurement of microwave current; measurement of microwave power; measurement of microwave voltage; mismatch error; picosecond rise-time pulse evaluation; power measurement; pulse-rise-time standardization; sampling oscilloscope standardization; spectrum analyzer standardization; termination mismatch error elimination; thin-film bolometers; voltage measurement.

A novel device—the BOLOVAC—is employed in measurement systems that furnish known voltages and currents up to 18 GHz, remove serious difficulties in power measurements, and are applicable in impedance, attenuation and other measurements. Typical of such measurements are the evaluation of rf power sources; calibration of power meters; measurement of net and incident power flow in a system; calibration of signal genera-

tors, voltmeters, current meters, picosecond-rise-time pulse-display oscilloscopes, spectrum analyzers; determination of insertion loss of components; and calibration of directional couplers. The Bolovac also serves as an accurately known resistive termination for match or mismatch applications from LF through microwaves.

Monogr. 124. **Reference tables for low-temperature thermocouples**, L. L. Sparks, R. L. Powell, and W. J. Hall, Nat. Bur. Stand. (U.S.), Monogr. 124, 61 pages (June 1972).

Key words: Cryogenics; homogeneity tests; liquid helium; liquid hydrogen; liquid nitrogen; thermocouples.

The experimental program to establish low-temperature reference tables for the commonly used thermocouples has been completed. Details of the experimental system, instrumentation, data analysis, error analysis, and materials tested are given in order to allow the user to better evaluate and apply the results. The results presented here include: (1) Reference tables for thermocouple types E, K, and T, both as  $E=f(T)$  and  $T=f(E)$ . The shorter  $f(E)$  tables have a 0 °C (273.15 K) reference temperature while all other tables have a 0 K reference temperature; (2) Reference tables for Pt and Ag-28 at% Au vs the materials used in thermocouple types E, K, and T. These data are presented as  $E=f(T)$  only; (3) Orthogonal polynomials and the associated coefficients necessary to generate the data with reduced order approximations; and (4) Power series coefficients for full precision reproduction of the reference data.

The data presented in the  $E=f(T)$  tables cover the temperature range from 0 to 280 K. The  $T=f(E)$  tables cover temperature ranges from 273.15 K down to the lowest temperatures allowed by table resolution.

Monogr. 127. **NBS papers on underground corrosion of steel piling 1962-1971. Corrosion of steel pilings in soils, corrosion evaluation of steel test piles exposed to permafrost soils, performance of steel pilings in soils, and polarization measurements as related to corrosion of underground steel piling**, W. J. Schwerdtfeger and M. Romanoff, Nat. Bur. Stand. (U.S.), Monogr. 127, 63 pages (Mar. 1972).

Key words: Active region; aerated soil; corrosion; disturbed soil; excavated; extracted; H-piling; instantaneous corrosion rate; mill scale; permafrost region; pipe piling; pit depth; polarization; sheet piling; undisturbed soil; weight loss.

This monograph is a collection of published papers on underground corrosion of steel piling. The papers are as follows: (1) Romanoff, Melvin, Corrosion of Steel Pilings in Soils, Nat. Bur. Stand. (U.S.), Monogr. 58, (Oct. 1962); (2) Romanoff, Melvin, Corrosion Evaluation of Steel Test Piles Exposed to Permafrost Soils, Proceedings 25th Conference, National Association of Corrosion Engineers, page 6 (Mar. 1969); (3) Romanoff, Melvin, Performance of Steel Pilings in Soils, Proceedings 25th Conference, National Association of Corrosion Engineers, page 14 (Mar. 1969); (4) Schwerdtfeger, W. J., Polarization Measurements as Related to Corrosion of Underground Steel Piling, J. Res. Nat. Bur. Stand. (U.S.), 75C (Eng. and Instr.) No. 2, 107-121 (Apr.-June 1971).

The papers describe corrosion of various types of steel piling exposed underground in the United States under climatic conditions ranging from semi-tropical to frigid. Corrosion is described



on driven piling above and below the water table after many years of exposure in soils having resistivities between 78 and 50,000 ohm-cm and ranging in pH from 2.3 to 8.8.

One of the papers demonstrates the value of a polarization technique in measuring corrosion. Polarization data were obtained on weighed steel pipe specimens exposed underground for seven years in backfilled soil trenches in the vicinity of driven sheet piling. The technique was evaluated by comparing calculated cumulative weight losses of specimens with their actual weight losses. The technique was also shown to be applicable to underground pipe piling. Supersedes NBS Monograph 58.

Monogr. 128. **Corrosion rates on underground steel test piles at Turcot Yard, Montreal, Canada—Part 1**, W. J. Schwerdtfeger and M. Romanoff, Nat. Bur. Stand. (U.S.), Monogr. 128, 17 pages (July 1972).

Key words: Average penetration rate; H-piles; instantaneous corrosion rate; linear polarization; pit depth; polarization curve.

In 1966, isolated steel H-piles allocated for underground corrosion tests were installed in three locations at the Turcot Yard Interchange of the Transcanadian Highway at Montreal. The reason for the installation was to furnish answers to some questions concerning the corrosion characteristics of piles, 12 in-74 lb/ft (30.5 cm-110 kg/m), which are identical with the piles supporting the concrete piers under the highway. Polarization measurements have been made once every year since installation.

This paper describes the determination of corrosion rates based on the polarization measurements made up to the time of removal of the first group of piles in 1969. The piles, placed underground at the three locations, differ mainly in that at one site all the piles are bare, at the second site the upper ends of the piles are coated with an epoxy paint and at the third site the upper ends are encased in concrete. Physical measurements made on the cleaned piles after removal are correlated with corrosion

rates calculated from the polarization measurements. Also, penetration rates on the piling based on the polarization data are compared with average penetration rates (based on actual weight losses) on relatively small pipe specimens. The pipe specimens were removed from 28 underground sites having a range of soil resistivities comparable to those of the three piling sites.

Using one of the polarization techniques applied to the individual test piles, polarization measurements were also carried out on 32 interconnected piles supporting one of the concrete piers. The calculated average corrosion rate of the 32 piles was found to compare favorably with that of the separate test piles in the same area.

Monogr. 129. **The development of Loran-C navigation and timing**, G. Hefley, Nat. Bur. Stand. (U.S.), Monogr. 129, 144 pages (Oct. 1972).

Key words: Cyclan; cytac; Loran; Loran-C; low frequency; navigation; pulse propagation; radio positioning; time dissemination; time transfer system.

The Loran-C timing and navigation concept and its implementation in the form of the Loran-C system has taken on considerable importance in a variety of military and civilian applications such as microsecond clock synchronization, precision tactical or civil navigation, etc. Future applications like tying together continental surveys, aircraft collision avoidance, etc., have yet to be explored in detail. This work traces the development of the Loran-C concept from its inception as a 100 kHz pulse hyperbolic navigation system to more recent times when it found a variety of applications to both timing and navigation. This work is intended to present the story of Loran-C in a readable and understandable way without resorting to the complicated mathematical formulation of the theory or detailed instrumentation aspects. Thus, the history, experimental and theoretical developments, political decisions, and field testing of the early equipment are described and the lessons learned can certainly be a guide for modern development of the system in all its detailed applications.

### 3.5. HANDBOOKS

Recommended codes of engineering and industrial practice (including safety codes) developed in cooperation with interested industries, professional organizations, and regulatory bodies. In many cases recommended requirements are given official status through their incorporation in local ordinances by State and municipal regulatory bodies.

**H105-1 (Revised 1972). Specifications and tolerances for reference standards and field standard weights and measures. 1. Specifications and tolerances for field standard weights (NBS class F),** T. M. Stabler, Nat. Bur. Stand. (U.S.), Handb. 105-1, 12 pages (July 1972).

Key words: Field standard weights; specifications; test weights; tolerances; weights and measures inspection; weights used by servicemen.

These specifications and tolerances are recommended as minimum requirements for standards used in the field by State and local weights and measures officials in examination of weighing devices. Revision of NBS Handbook 105-1, April 1969.

**H109. Aluminum wire tables,** C. Peterson, J. L. Thomas, and H. Cook, Editors, Nat. Bur. Stand. (U.S.), Handb. 109, 66 pages (Feb. 1972).

Key words: Aluminum conductor; aluminum wire cables; conversion factors; electrical conductivity; electrical conductor; electrical resistivity; standard values; temperature coefficient.

This handbook of aluminum wire tables is a companion publication to NBS Handbook 100, Copper Wire Tables, a review of which is contained in Part I, Sections 1 and 2. Data are presented on the conductivities and resistivities of both solid and stranded wires of various sizes and composition, together with a variety of other data of interest to the designer of electrical equipment and installations. Values are expressed in both U.S. Customary and International System (SI) Units. Wire sizes involved are based on and restricted to those manufactured and typically used in the United States. American Wire Gage sizes are used for the smaller range of conductors from 56 gage through 4/0. Larger conductors are sized on the basis of circular mil area. The alloy compositions included in these tables are EC-

0 (annealed), EC-H19, 5005-H19, and 6201-T81; values are given over a temperature range of 0 to 100 °C.

**H110-1. National Electrical Safety Code. Part 1. Rules for the installation and maintenance of electrical supply stations and equipment,** Nat. Bur. Stand. (U.S.), Handb. 110-1, 43 pages (June 1972).

Key words: Electrical safety; electrical supply station; electrical utility station; high voltage safety; power station equipment; power station safety.

This Handbook contains Part 1 of the National Electrical Safety Code and supersedes NBS Handbook H31 and pages 31 through 75 of the NBS Handbook H30. Part 1 of this Code covers the electric conductors and equipment in electrical supply stations along with the associated structural arrangements employed, for example, by an electrical or railway utility in the exercise of its function as a utility and accessible only to properly qualified personnel. It also covers similar electric conductors and equipment in electrical supply stations when owned by and installed in an industrial establishment, where the electrical supply stations are under the control of and accessible only to properly qualified persons. Examples of such industrial establishments are the paper and steel industries.

**H111. American National Standard. Radiation safety for x-ray diffraction and fluorescence analysis equipment,** Nat. Bur. Stand. (U.S.), Handb. 111, 20 pages (June 1972).

Key words: Radiation safety; x-ray equipment.

This standard reviews the types of injuries resulting from accidental exposure to ionizing radiation resulting from the operation of x-ray diffraction and fluorescence analysis equipment, establishes equipment design criteria, sets up requirements for approved operating procedures and recommends the establishment of health surveillance, and personnel monitoring programs. The circumstances under which operation of equipment must be limited to specially designated areas equipped with radiation barriers and warning signs are set forth. Maximum permissible dose limits established by the National Council on Radiation Protection and Measurement are stated. A list of references to selected articles on various aspects of radiation safety is given and notes on the detection and measurement of radiation from x-ray diffraction and fluorescence analysis equipment are included in an appendix.



### 3.6. SPECIAL PUBLICATIONS

This series includes proceedings of high-level national and international conferences sponsored by NBS, precision measurement and calibration volumes, NBS Research Highlights, and other special publications appropriate to this grouping, such as administrative pamphlets, wall charts and bibliographies.

**SP236, 1972 Edition. NBS Frequency and time broadcast services, radio stations WWV, WWVH, WWVB, and WWVL, P. P. Vitzbicke, Editor, Nat. Bur. Stand. (U.S.), Spec. Publ. 236, 14 pages (Mar. 1972).**

**Key words:** Broadcast of standard frequencies; high frequency; low frequency; standard frequencies; time signals; very low frequency.

Detailed descriptions are given of the technical services provided by the National Bureau of Standards radio stations WWV, WWVH, WWVB, and WWVL. These services are: 1. Standard radio frequencies; 2. Standard audio frequencies; 3. Standard musical pitch; 4. Standard time intervals; 5. Time signals; 6. UT1 corrections; and 7. Official announcements. In order to provide users with the best possible services, occasional changes in broadcasting schedules are required. This publication shows the schedules in effect on January 1, 1972. Annual revisions will be made. Current data relating to standard frequencies and time signals are available monthly in the Time and Frequency Services Bulletin. Advance notices of changes occurring between revisions will be sent to users of NBS broadcast services who request such notice on the basis of need. (Supersedes NBS Special Publication 236, 1971 and previous editions.)

**SP260-24. Standard reference materials: comparison of redox standards, K. M. Sappenfield, G. Marinenko, J. L. Hague, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-24, 97 pages (Jan. 1972).**

**Key words:** Analytical procedures; arsenic-iodine method; comparison; effective purity; oxidimetric standards.

The methods described in this publication are those that have been used at the National Bureau of Standards for the comparison of the current oxidimetric standard reference materials with each other and for the determination of the effective purity of these standard reference materials. The methods, which are modifications of well-established and previously published methods, were selected or designed for their accuracy and dependability. An accurate method was devised for the determination of the effective purity of the arsenic trioxide standard SRM 83c by adding solid iodine and determining the excess iodine photometrically.

**SP260-33. Standard reference materials: comparison of original and supplemental SRM 705, narrow molecular weight distribution polystyrene, H. L. Wagner, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-33, 30 pages (May 1972).**

**Key words:** Characterized polymers; narrow molecular weight polystyrene; polystyrene standard; Standard Reference Material 705.

Because the supply of the original batch of narrow molecular weight distribution polystyrene, SRM 705, is almost exhausted, another supply of polystyrene, reported to be from the same batch as the original has been characterized to determine whether it is the same as the original as far as the properties listed on the certificate are concerned. No difference in molecular weight as measured by light scattering, osmometry, or gel-

permeation chromatography could be found. The limiting viscosity numbers were also the same. It was also shown from solution viscosity measurements that pellet to pellet variation in molecular weight is negligible.

**SP260-34. Standard reference materials: thermoelectric voltage of silver-28 atomic percent gold thermocouple wire, SRM 733, versus common thermocouple materials (between liquid helium and ice fixed points), L. L. Sparks and J. G. Hust, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-34, 34 pages (Apr. 1972).**

**Key words:** Cryogenics; Seebeck voltage; silver-gold alloy; Standard Reference Material; thermocouple.

Industry wide standardization of thermocouple wire depends, in part, on the ability to thermoelectrically compare commercial wires with a Standard Reference Material (SRM). The alloy Ag-28 at% Au, SRM 733, meets the requirements of a thermoelectric reference material, particularly in the temperature range of liquid helium and liquid hydrogen where Pt-67 is not adequate. Thermoelectric voltage comparisons are reported for SRM 733 versus common thermocouple materials between liquid helium and ice fixed points. Detailed standard reference data based on these common materials are given in NBS Monograph 124. The comparisons were made in a thermocouple comparator which was designed to be a permanent holder of three SRM 733 wires; the comparator allows tests to be made without handling the standard wires. Details of the construction, testing, and analysis of the comparators are given.

**SP260-35. Standard reference materials: thermal conductivity of austenitic stainless steel, SRM 735, from 5 to 280 K, J. G. Hust and L. L. Sparks, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-35, 22 pages (Apr. 1972).**

**Key words:** Cryogenics; electrical resistivity; stainless steel; Standard Reference Material; thermal conductivity.

Thermal conductivity data are presented for a well-characterized austenitic stainless steel. Thermal conductivity and electrical resistivity measurements were conducted on two lots of this steel. Electrical resistivity measurements were performed on the second lot both before and after the material was hot-swaged and reannealed to a size 1/10 the original diameter. These measurements indicate that this steel can be swaged and reannealed without an appreciable change in thermal conductivity. Electrical resistivity measurements as well as direct thermal conductivity measurements on several specimens from both lots indicate a material variability in these lots of less than 1% in thermal conductivity.

**SP260-36. Standard reference materials: a referee method for the determination of calcium in serum, J. P. Cali, J. Mandel, and L. Moore, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-36, 136 pages (May 1972).**

**Key words:** Accuracy; atomic absorption spectrometry; calcium in serum; clinical chemistry; referee method for calcium.

The first referee method of analysis (a method of known accuracy) in clinical chemistry has been developed by a team of experts from clinical chemistry, 8 cooperating clinical chemistry laboratories, and scientists from the National Bureau of Standards. Subject to the limitations and provisos stated, calcium in serum can be determined by the referee method to within  $\pm 2\%$  of the "true or absolute" value. Also discussed are: (1) What



Constitutes a Meaningful Measurement System; (2) Theory of Operation and Practice Required to Develop a Referee Method; (3) History of the Actual Work; the Referee Method Protocol; (4) Results; (5) The Isotope-Dilution Mass Spectrometry Work; (6) Discussion, Conclusions, and Recommendations for Future Referee Method Developments.

**SP260-37. Standard reference materials: methods of analysis of NBS clay standards,** J. I. Shultz, R. K. Bell, T. C. Rains, and O. Menis, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-37, 86 pages (June 1972).

**Key words:** Atomic absorption; ceramics; classical procedures; clay materials; flame emission; refractories; Standard Reference Materials.

This publication brings together a compilation of methods used at NBS for the analysis of two complex standard reference clay materials. The methods were selected to give the best obtainable results for those elements normally found in clays. In some instances, more than one procedure was employed for an element as a cross-check on the precision and accuracy of the results. The procedures are presented in two parts. Part I is concerned with the determination of the major constituents by the classical analytical procedures. Part II covers the minor elements which are determined instrumentally by flame emission and atomic absorption spectrometry. These clay materials serve as analytical composition standards to provide quality control of the basic raw materials which are used in the ceramics and refractories industries.

**SP260-38. Standard reference materials: preparation and calibration of standards of spectral specular reflectance,** J. C. Richmond and J. J. Hsia, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-38, 57 pages (May 1972).

**Key words:** Aluminum; gold; infrared reflectance; interferometer; mirrors; reflectance; reflectance standards; spectral reflectance; spectral specular reflectance; specular reflectance; standards; ultraviolet reflectance.

This report describes in detail the preparation and calibration of Standard Reference Materials 2001 through 2008. These standards of spectral specular reflectance were prepared commercially by vacuum depositing opaque coatings of gold and aluminum, respectively, onto polished substrates of fine-annealed borosilicate glass. The near-normal ( $9^\circ$  from normal) spectral specular reflectance was measured by the multiple-reflection technique. Four different combinations of source, spectrometer, and detector were used to cover the wavelength range from about  $0.25\ \mu\text{m}$  to  $30\ \mu\text{m}$  and beyond.

**SP260-39. Standard reference materials: the eddy current decay method for resistivity characterization of high purity metals,** A. F. Clark, V. A. Deason, J. G. Hust, and R. L. Powell, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-39, 53 pages (May 1972).

**Key words:** Apparatus; characterization; eddy current decay; electrical resistivity; high purity metals; homogeneity; low temperature.

Characterization of high purity metals by resistivity measurements at low temperatures is discussed. In particular, the eddy current decay method of resistivity measurement is described in detail. The advantages and limitations are presented along with the theoretical basis of the method. Detailed instructions are given for constructing and operating the apparatus.

**SP260-40. Standard reference materials: selection of differential thermal analysis temperature standards through a cooperative study (SRM 758, 759, 760),** H. G. McAdie, P. D. Garn, and O. Menis, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-40, 71 pages (Aug. 1972).

**Key words:** DTA; International Confederation on Thermal Analysis; international cooperative testing; Standard Reference Materials NBS 758, 759, 760; temperature scale; thermal analysis.

The testing and evaluation program leading to the certification of 10 materials as Standard Reference Materials NBS 758, 759 and 760, for calibrating the temperature scale for thermal analysis is described. The international cooperative testing program was set up on the basis of a preliminary program initiated in 1966. Thirty-four laboratories reported to the Standards Committee of the International Confederation on Thermal Analysis. The results were obtained on a variety of apparatus under their conditions of experimentation, except that the heating rate was prescribed in the range of 4 to  $10^\circ\text{C}$  per minute. The data were processed to obtain means and measures of scatter, not only in total, but separated in terms of a number of sample number of sample holder parameters. The sample holder geometry was the only parameter having a clear effect on the extrapolated onset and peak temperatures. The effects of the thermocouple position and calibration were tested, but no significant effect was found. The heating rate has only a small effect, tending to increase the spread of onset and peak temperature values from the DTA are somewhat higher than the thermodynamic equilibrium values reported in the literature. Based on the mean values from all the laboratories the standard deviation was  $5$  to  $8^\circ\text{C}$ , which includes the bias between laboratories as well as measurement errors.

**SP260-41. Standard reference materials: use of standard light-sensitive paper for calibrating carbon arcs used in testing textiles for colorfastness to light,** L. A. Wood and P. J. Shouse, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-41, 24 pages (Aug. 1972).

**Key words:** Carbon-arcs, standardization of; color-fastness, testing of; fading tests, standardization; light-sensitive paper; paper, light-sensitive; textiles, fading of.

The use of NBS Light-Sensitive Paper and NBS Booklets of Standard Faded Strips in the standardization of carbon arcs is described. These lamps are used to determine the fading characteristics and degradation of textiles and other materials when subjected to visible and ultraviolet radiation. The light-sensitive paper is useful in calibrating the arcs in terms of NBS Standard Fading Hours (SFH) or equivalent exposure in the NBS Master Carbon-Arc Lamp.

**SP260-42. Standard reference materials: the characterization of linear polyethylene SRM 1475,** H. L. Wagner and P. H. Verrier, Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 260-42, 39 pages (Sept. 1972).

**Key words:** Density; differential refractive index; gel permeation chromatography (GPC); light scattering; linear polyethylene; melt flow rate; molecular weight distribution; number average molecular weight; osmometry; refractive index; standard reference material; viscosity; weight average molecular weight; Z average molecular weight.

The National Bureau of Standards has issued a linear polyethylene standard reference material, SRM 1475. This material is certified for weight average molecular weight ( $M_w$ ), number average molecular weight ( $M_n$ ), Z average molecular weight ( $M_z$ ), molecular weight distribution, limiting viscosity numbers in several solvents, melt flow rate, and density. The experimental details of the determination and certification of these properties are given in these collected papers previously published in the Journal of Research of the National Bureau of Standards.

**SP260-43. Standard reference materials: preparation and homogeneity characterization of an austenitic iron-chromium-nickel alloy,** H. Yakowitz, A. W. Ruff, and R. E. Michaelis,

Nat. Bur. Stand. (U.S.), Spec. Publ. 260-43, 19 pages (Nov. 1972).

**Key words:** Austenitic stainless steel; electron probe microanalysis; Fe-Cr-Ni alloy; homogeneity testing; metallography; stacking fault energy; Standard Reference Material.

An alloy of weight fraction 0.710 iron, 0.183 chromium and 0.107 nickel was characterized at the micrometer level of spatial resolution by means of electron probe microanalysis. This alloy, designated SRM 479, is of suitable homogeneity for use as a standard in microanalytical techniques. The coefficient of variation for each of the three elements is not more than 1.5% based on about 800 analyses involving five different specimens. There is no statistically significant variation in composition within specimens or from specimen to specimen. Electron probe microanalysis was carried out using different instrumental conditions and operators. SRM 479 is supplied as a disc about 4.6mm diameter by 1mm thick.

**SP260-44. Standard reference materials: preparation and use of superconductive fixed point devices, SRM 767, J. F. Schooley, R. J. Soulen, Jr., and G. A. Evans, Jr., Nat. Bur. Stand. (U.S.), Spec. Publ. 260-44, 35 pages (Dec. 1972).**

**Key words:** Aluminum; cadmium; cryogenics; indium; lead; magnetic susceptibility; superconductive transition temperature; superconductivity; thermometric fixed points; zinc.

The preparation, testing, and use of SRM 767 devices are described. These devices incorporate samples of lead, indium, aluminum, zinc, and cadmium within a mutual inductance coil pair. These elements become superconductive at temperatures near 7.2, 3.4, 1.2, 0.85 and 0.5 K, respectively, and the transition midpoints, when attained by observing the sample magnetic susceptibilities in negligible small magnetic fields, provide thermometric reference points which are reproducible to  $\pm 1$  mK.

**SP300. Volume 5. Precision measurement and calibration. Selected NBS papers on frequency and time, B. E. Blair and A. H. Morgan, Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 300, Vol. 5, 565 pages (June 1972).**

**Key words:** Atomic beams; atomic clocks; atomic standards; atomic time; clock synchronization; coordinated U.T. dissemination of frequency and time; flicker noise; frequency and time standards; frequency measurement; frequency stability; international comparison of atomic standards; lasers; masers; radio frequency measurements; satellite timing; spectral density; standard frequency and time broadcasts; statistics of frequency and time measurements; time scales; time synchronizations; TV timing; VLF timing.

This is one of a series of volumes consisting of a group of selected papers and monographs by NBS authors, and abstracts of papers by non-NBS and NBS authors, dealing with the precision measurement of specific physical quantities and related topics. The contents should be useful to those in the scientific community who are engaged in frequency and time measurements or are otherwise interested in these physical quantities.

This volume contains selected reprints, and abstracts of very general papers, printed in chronological order in most cases from January 1960 through June 1969, covering the following general topics: Frequency and Time Standards, Time Scales, Distribution of Frequency and Time Signals, Statistics of Frequency and Time Standards, and Selected Frequency and Time References.

**SP300. Volume 8. Precision measurement and calibration. Selected NBS papers on mechanics, R. L. Bloss and M. J. Orloski, Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 300, Vol. 8, 590 pages (Jan. 1972).**

**Key words:** Acoustics; fluid mechanics; force; gravity; humidity; pressure; strain; vacuum; vibration; viscosity.

This volume is one of an extended series which brings together the previously published papers, monographs, abstracts, and bibliographies by NBS authors dealing with the precision measurement of specific physical quantities and the calibration of the related metrology equipment. The contents have been selected as being useful to the standards laboratories of the United States in tracing to NBS standards the accuracies of measurement needed for research work, factory production, or field evaluation.

Volume 8 consists primarily of published works of the staff of the Mechanics Division of NBS. It includes papers in the fields of acoustics, fluid mechanics, force, gravity, humidity, pressure, strain, vacuum, vibration, and viscosity. Although most of the papers had been previously published, original papers in the fields of "gravity" and "viscosity" are included.

**SP300. Volume 9. Precision measurement and calibration. Selected NBS papers on colorimetry, I. Nimeroff, Editor, Nat. Bur. Stand. (U.S.), Spec. Publ. 300, Vol. 9, 460 pages (June 1972).**

**Key words:** Appearance evaluation; colorimetry; color spacing; color vision; gloss; metamerism; spectrophotometry; standards; uncertainty; variability.

This volume is one of an extended series which brings together the previously published papers, monographs, abstracts, and bibliographies by NBS authors dealing with the precision measurement of specific physical quantities and the calibration of the related metrology equipment. The contents have been selected as being useful to the standards laboratories of the United States in tracing to the NBS standards the accuracies of measurement needed for research work, factory production, or field evaluation.

Volume 9 treats the field of Colorimetry. It contains 37 reprints on Colorimetry and Spectrophotometry assembled in 8 sections: (1) Spectrophotometry, (2) Color Vision, (3) Color Specification, (4) Sources and Instrumentation, (5) Color Spacing and Metamerism, (6) Variabilities and Uncertainties, (7) Appearance and Gloss, (8) List of Publications, LP39 (in part), Colorimetry and Spectrophotometry Publications by the Staff of the National Bureau of Standards, January 1957 through August 1969.

**SP304, Revised October 1972. The modernized metric system — The international system of units (SI), Nat. Bur. Stand. (U.S.), Spec. Publ. 304, 1 chart (Oct. 1972).**

**Key words:** International system of units; measurement systems; metric system; modernized metric system; SI; weights and measures.

The seven base units of the modernized metric system (also called the International System of Units, abbreviated SI), two supplementary units, several derived units, a meter stick and, for purposes of comparison, a yardstick are all shown on this four-color wall chart. Additional information shown includes a brief statement on the nature of the modernized metric system and its use in the United States, a table permitting conversion of commonly used units from SI to customary units and vice versa, and a table listing the names and symbols of decimal multiples and submultiples used with SI units.

**SP304A, Revised October 1972. Brief history of measurement systems with a chart of the modernized metric system, Nat. Bur. Stand. (U.S.), Spec. Publ. 304A, 4 pages (Oct. 1972).**

**Key words:** International system of units; measurement systems; metric system; modernized metric system; SI; weights and measures.



The Modernized Metric System (also called the International System of Units) is made up of seven base units, two supplementary units, and many derived units. The chart describes this entire system, including details about the standards for each base unit and information on how the system is used.

The reverse side of the chart contains a brief history of measurement systems. The need for measurement began with primitive man, who used parts of his body and his natural surroundings for measurement standards and measuring instruments. As societies evolved, weights and measures became more complex. Two systems became predominant: the English system, rooted in the history and tradition of England; and the metric system, a scientifically based system using decimal notation. The metric system, with its inherent decimal advantages, gained widespread acceptance and is now the official measurement system in nearly all countries of the world.

SP305. Supplement 3. **Publications of the National Bureau of Standards 1971 catalog. A compilation of abstracts and key word and author indexes**, B. L. Oberholtzer, Nat. Bur. Stand. (U.S.), Spec. Publ. 305 Suppl. 3, 342 pages (July 1972).

Key words: Abstracts, NBS publications; key words; publications.

This supplement to Special Publication 305 Supplements 1 and 2 the National Bureau of Standards lists the publications of the Bureau issued between 1 January 1971 and 31 December 1971. It includes an abstract of each publication (plus some earlier papers omitted from Special Publication 305 Supplement 2), key-word and author indexes; and general information and instructions about NBS publications.

Miscellaneous Publication 240 (covering the period July 1, 1957 through June 30, 1960) and its supplement (covering the period July 1, 1960 through June 30, 1966), Special Publication 305 (covering the period July 1966 through December 1967) and Special Publication 305 Supplement 1 (covering the period 1968-1969), and Special Publication 305 Supplement 2 (covering the period 1970), remain in effect. Two earlier lists, Circular 460 (Publications of the National Bureau of Standards, 1901 to June 1947) and its supplement (Supplementary List of Publications of the National Bureau of Standards, July 1, 1947 to June 30, 1957) are also still in effect. To accompany National Bureau of Standards Circular 460; its Supplement, Miscellaneous Publication 240; its Supplement, Special Publication 305; and its Supplements 1 and 2.

SP323. **Electronic density of states**. Based on invited and contributed papers and discussion, 3d Materials Research Symposium held at Gaithersburg, Md., Nov. 3-6, 1969, L. H. Bennett, Editor, Nat. Bur. Stand. (U.S.), Spec. Publ. 323, 834 pages (Dec. 1971).

Key words: Band structure; disordered systems; electronic density of states; ion neutralization; Knight shift; magnetic susceptibility; many-body effects; optical properties; photoemission; soft x-ray; specific heat; superconductivity; transport properties; tunneling.

This volume is based on materials presented at the Third Materials Research Symposium of the National Bureau of Standards, held November 3-6, 1969. It provides a review of various experimental and theoretical techniques applied to the study of the electronic density of states in solids and liquids. The topics covered in a series of invited and contributed papers include theory of and experiments to obtain the one-electron density-of-states; many-body effects; optical properties; spectroscopic methods such as photoemission (x-ray and UV), ion neutralization, and soft x-ray; obtaining the density-of-states at the Fermi level by specific heat, magnetic susceptibility, and the Knight

shift; the disordered systems of alloys, liquids, dirty semiconductors, and amorphous systems; and superconducting tunneling and the application of density of states to properties such as phase stability.

An edited discussion follows many of the papers. *These proceedings include the following papers (indented):*

**The band structure problem**, J. M. Ziman, *SP323*, pp. 1-12 (Dec. 1971).

Key words: APW; band structure; density of states; disordered systems; KKR; *t*-matrix; molecular crystals; pseudopotential.

The numerical solution of the Schrödinger equation for an electron in a dense assembly of atoms (*i.e.* a solid or liquid metal or semiconductor) has made great progress in the past ten years. This is not merely a consequence of greater computing power; we now have a much better grasp of the mathematical theory of such solutions.

By 1960 a number of practical methods had been devised for the computation of the electronic structure of ordered crystals, but these lacked intuitive interpretation. The first advance was to rewrite the OPW method in terms of pseudopotentials, thus making sense of the free-electron theory of metals. This development has proved particularly valuable in semiquantitative and empirical investigations of Fermi surfaces, transport properties, lattice dynamics, cohesion, *etc.*, but we have had to wait until recently for a rigorous analysis of the criteria for convergence of the various types of model potential or pseudopotential that have been postulated.

The next step was to show that the KKR (Green function) method could also be expressed as a pseudopotential, and then to demonstrate that this was also a form of APW expansion. The relative computational power of these two methods can thus be analyzed, and questions answered concerning the fulfillment of the empty lattice test, the apparent lack of uniqueness of the expansions, the advantages of "folding" matrix elements from distant points of the reciprocal lattice, and the introduction of contributions from the interstitial potential.

At this stage, the connections between the band structure problem and the *t*-matrix theory of scattering were uncovered, and *d*-bands were seen to arise as resonances of the muffin-tin wells. The KKR matrix could now be rewritten as a mixture of pseudopotential and tight-binding elements, in harmony with the empirical model Hamiltonian representations of hybridised *s-p* and *d*-bands. This method not only permits more rapid computations, but shows clearly how the width and position of such bands should depend on the atomic potential.

Some problems still remain. For example, present techniques do not seem adequate for first-principles calculations on molecular crystals, where the anisotropy of the interstitial potential (*i.e.* easy channels along bonds, but high hills between layers or chains) is probably the dominant feature.

As for disordered systems — we know little for certain and nothing quantitatively. The linear chain model has been fully studied but is quite irrelevant to the three-dimensional case. The present theoretical confusion is exemplified by the equiconcentration substitutional alloy in the tight-binding limit; some formulae give only one band, others allow two. Again, the very possibility of producing band gaps by diffraction of free electrons in a topologically disordered system (*e.g.* amorphous Ge) has not been demonstrated mathematically with any rigor.



**Electronic density of states of transition, noble, and actinide metals**, F. M. Mueller, *SP323*, p. 17 (Dec. 1971).

Key words: Electronic density of states; histogram representations; QUAD scheme.

**Electronic densities of states and optical properties of CsCl type intermetallic compounds**, J. W. D. Connolly and K. H. Johnson, *SP323*, pp. 19-25 (Dec. 1971).

Key words: AuZn; CsCl-type intermetallic compounds; direct interband transitions; electronic density of states; NiAl; optical properties.

The electronic band structures and densities of states have been calculated from first principles for two intermetallic compounds having the CsCl structure. The non-relativistic augmented plane wave method has been used in conjunction with an LCAO interpolation technique to determine the band structure and density of states of  $\beta'$ -NiAl to a high degree of accuracy. These theoretical results are in excellent agreement with the measured optical properties if  $k$ -conserving (direct) interband transitions are assumed to be dominant. A similar study has been carried out for  $\beta'$ -AuZn, using as a basis the energy bands determined by the relativistic Korringa-Kohn-Rostoker method. The band profiles and density of states of  $\beta'$ -AuZn are qualitatively similar to those of  $\beta'$ -NiAl, except for the appearance of relativistic effects in the former alloy and differences in the relative positions and widths of the respective Au and Ni  $d$ -bands. The  $\beta'$ -AuZn results have also been compared with the measured optical properties and are again consistent with these measurements if direct interband transitions are assumed.

**The calculation of densities of states by LCAO interpolation of energy bands with application to iron and chromium**, J. W. D. Connolly, *SP323*, pp. 27-32 (Dec. 1971).

Key words: Chromium; electronic density of states; interpolation method; iron; photoemission.

The LCAO (linear combination of atomic orbitals) interpolation method is described as a means of calculating the density of states curves of a crystalline solid. This method is shown to be more straightforward and convenient to use than the composite (LCAO-OPW) techniques that have recently been proposed for transition metals. A computer program is described which determines the LCAO interaction integrals from an *ab initio* energy band calculation by a nonlinear least squares procedure, and then uses these parameters to sample the Brillouin zone at a large number of points in order to calculate the density of states curve to a high degree of accuracy. As examples of the application of this program, the results of calculations on chromium (in both the nonmagnetic and antiferromagnetic states) and iron (nonmagnetic and ferromagnetic) are presented and compared with the recent photoemission data.

**Optical properties of aluminum**, G. Dresselhaus, M. S. Dresselhaus, and D. Beaglehole, *SP323*, pp. 33-36 (Dec. 1971).

Key words: Aluminum (Al); dielectric constant; electronic density of states; interband transition; optical properties; pseudopotential.

The Ashcroft energy band model which provides a good representation of the measured Fermi surface of aluminum is used here to calculate the optical properties. New reflectivity measurements in aluminum have also been carried out between  $2\mu$  and  $3000 \text{ \AA}$  using a sensitive continuous frequency scanning technique. A Kramers-Kronig analysis of the reflectivity data yields a frequency dependent dielec-

tric constant which is essentially in agreement with the results of the calculation. This comparison suggests that the optical properties of aluminum can be described in terms of a one-electron energy band model.

**On the optical properties and the density of states in arsenic**, R. W. Brodersen and M. S. Dresselhaus, *SP323*, pp. 39-44 (Dec. 1971).

Key words: Arsenic (As); electronic density of states; Fermi surface; interband transition; Landau levels; magneto-reflection.

The infrared reflectivity of arsenic is calculated and correlated with Fermi surface, magnetoreflexion and optical reflectivity measurements. These infrared properties are strongly affected by interband transitions across a small spin-orbit induced bandgap. The unusually large intensity of this interband transition for light incident along the trigonal direction is due to the simultaneous occurrence of a strong interband momentum matrix element and a large density of states. By considering this interband transition explicitly, good agreement is obtained with the experimental data of Riccius.

**Density of states and ferromagnetism in iron**, K. J. Duff and T. P. Das, *SP323*, pp. 47-52 (Dec. 1971).

Key words: Electronic density of states; ferromagnetism; iron; optical reflection; photoemission; x-ray emission.

The band structure of ferromagnetic iron has been calculated by a variational method using a basis of tight-binding functions and orthogonalized plane waves. Exchange matrix elements are evaluated without approximation by a local potential. Correlation effects are explicitly included. Histograms for the density of states are constructed and compared with photoemission and optical reflection and x-ray emission data. The calculation leads self-consistently to the observed magnetic moment. The relative importance of intra-atomic exchange and itinerancy to the origin of iron's ferromagnetism is discussed.

**Calculation of density of states in W, Ta, and Mo**, I. Petroff and C. R. Viswanathan, *SP323*, pp. 53-56 (Dec. 1971).

Key words: Electronic density of states; Fermi energy; molybdenum; photoemission; tantalum; tungsten.

Density of states curves were calculated for tungsten, tantalum and molybdenum from corresponding energy band structures obtained by a nonrelativistic APW calculation. The Fermi energy and the density of states at the Fermi energy were obtained for each material. The calculations were part of a study intended to calculate theoretical photoemission yield curves which could be compared with experimental results.

**Adjustment of calculated band structures for calcium by use of low-temperature specific heat data**, R. W. Williams and H. L. Davis, *SP323*, pp. 57-61 (Dec. 1971).

Key words: Calcium; de Haas-van Alphen; electronic density of states; low-temperature specific heat; pseudopotential; transition-metal behavior.

The electronic band structure of calcium has been studied theoretically by employing the Korringa-Kohn-Rostoker method. The crystal potentials used in our calculation were obtained by means of a standard superposition of free-atom charge densities.  $E_k$  vs  $k$  curves and the density of states at the Fermi energy were calculated for various potentials, with the measured low-temperature electronic specific heat coefficient,  $\gamma$ , being used as an empirical aid to adjust the

exchange portion of the crystal potential. The important feature of the potentials used is that they all give band structures which have definite *d*-band character in the vicinity of the Fermi surface. These *d* bands or their corresponding *d* scattering resonances vary rapidly in energy for small changes in the exchange, resulting in values of  $\gamma$  which are extremely sensitive to exchange.

**Fermi surface properties of the noble metals at normal volume and as a function of pressure**, W. J. O'Sullivan, A. C. Switendick, and J. E. Schirber, *SP323*, pp. 63-65 (Dec. 1971).

Key words: Crystal potential; effective masses; electronic density of states; electronic specific heat; noble metals; pressure effects.

We present the results of nonrelativistic KKR calculations of the Fermi surface properties of Cu, Ag, and Au at normal volume and as a function of pressure. In particular we compare electronic specific heats, effective masses and the associated pressure shifts with the corresponding experimental results for the noble metals. In contrast to the results of previous calculations we find that the Herman-Skillman-Mattheiss crystal potential is an excellent effective potential for both Cu and Ag.

**Calculated effects of compression upon the band structure and density of states of several metals**, E. A. Kmetko, *SP323*, pp. 67-73 (Dec. 1971).

Key words: Alkali and alkaline earth metals; augmented plane wave method (APW); cerium; compressibility; electronic density of states; lanthanides.

Energy bands were obtained self-consistently by the augmented plane wave method for the following metals: Li, Cs, Ca, Sr, Ba, La, Ce, U, Pu, W and Fe. The density of states and the electronic charge were resolved into *s*-, *p*-, *d*-, and *f*-like components. Under compression the charges associated with the higher values of  $\ell$  increase, mainly at the expense of the *s*-like component, and a more compact overall distribution is thereby achieved. The present results indicate that such "electronic transitions" are of general occurrence and probably play a significant role in determining the compressibility of metals.

**Optical properties and electronic density of states**, M. Cardona, *SP323*, pp. 77-89 (Dec. 1971).

Key words: Critical points; density of states; dielectric constant; modulated reflectance; optical absorption.

The fundamental absorption spectrum of a solid yields information about critical points in the optical density of states. This information can be used to adjust parameters of the band structure. Once the adjusted band structure is known, the optical properties and the density of states can be generated by numerical integration. We review in this paper the parametrization techniques used for obtaining band structures suitable for density of states calculations. The calculated optical constants are compared with experimental results. The energy derivative of these optical constants is discussed in connection with results of modulated reflectance measurements. It is also shown that information about density of empty states can be obtained from optical experiments involving excitation from deep core levels to the conduction band.

A detailed comparison of the calculated one-electron optical line shapes with experiment reveals deviations which can be interpreted as exciton effects. The accumulating experimental evidence pointing in this direction is reviewed together with the existing theory of these effects.

A number of simple models for the complicated interband density of states of an insulator have been proposed. We review in particular the Penn model, which can be used to account for response functions at zero frequency, and the parabolic model, which can be used to account for the dispersion of response functions in the immediate vicinity of the fundamental absorption edge.

**Theoretical electron density of states study of tetrahedrally bonded semiconductors**, D. J. Stukel, T. C. Collins, and R. N. Euwema, *SP323*, pp. 93-102 (Dec. 1971).

Key words: Aluminum phosphide (AlP); electronic density of states; exchange potential; gallium arsenide (GaAs); germanium; self-consistent orthogonalized plane wave model (SCOPW); semiconductors, tetrahedrally bonded; silicon; zincblende; ZnSe.

The electron density of states has been calculated using a self-consistent orthogonalized plane wave (SCOPW) model for compounds in the isoelectronic sequences Si-AlP and Ge-GaAs-ZnSe. The valence and conduction band density of states are presented. The location of the core states is also given. The effect upon the density of states of using the exchange approximations of Slater, Kohn-Sham, and Liberman is displayed.

**Electronic density of states in Eu-chalcogenides**, S. J. Cho, *SP323*, pp. 105-108 (Dec. 1971).

Key words: Augmented plane wave method (APW); electronic density of states; europium-chalcogenides; exchange potential; *f* bands; photoemission.

The spin-polarized energy bands and the electronic density of states in the Eu-chalcogenides have been obtained by the augmented-plane-wave (APW) method. The results show that the *f* bands are extremely sensitive to the exchange potential used, and the *f* ( $\uparrow$ ) bands become the highest valence bands with a band width of the order of 0.5 eV. Our results have been compared with the recent photoemission spectroscopy data. The UPS data show too large *f* band width and too small relative peak intensities of the *f* bands, which disagree with our results. The 4*f* bands in the Eu and Gd could be located within 3.0 eV below their Fermi energies.

**Energy band structure and density of states in tetragonal GeO<sub>2</sub>**, F. J. Arlinghaus and W. A. Albers, Jr., *SP323*, pp. 111-113 (Dec. 1971).

Key words: Augmented plane wave method (APW); electronic densities of states; GeO<sub>2</sub>; indirect transition; optical properties; Slater exchange; vacuum ultraviolet reflectance spectra.

The electronic energy bands of tetragonal GeO<sub>2</sub> have been calculated and correlated with optical properties of single crystals of this material. The agreement between theory and experiment is sufficiently good to warrant calculations of densities of states and conduction band effective masses preparatory to the determination of the dielectric constant as a function of energy. The calculated energy bands, density of states, and the experimental optical absorption edge data are presented and discussed.

**Calculation of the density of states and optical properties of PbTe from APW-LCAO energy bands**, D. D. Buss and V. E. Schirf, *SP323*, pp. 115-123 (Dec. 1971).

Key words: Augmented plane wave method (APW); electronic density of states; *k*-*p* method; LCAO; lead telluride (PbTe); optical properties; pseudopotential; random phase approximation; tight-binding.



The overlap integrals in the tight-binding secular equation for the relativistic  $p$ -bands in PbTe have been adjusted to give the best representation of the APW results at high symmetry points. The resulting LCAO bands have been used to calculate the density of states in energy and the optical constants of PbTe. The calculated density of states is found to have peaks which correspond closely to the four peaks measured by Spicer and Lapeyre. However, the assignment of peaks to bands is found to be different from that proposed previously. The method of Dresselhaus and Dresselhaus has been used to obtain the oscillator strengths for optical transitions, and these are found to agree with previous calculations. The interband electronic contribution to the optical constants has been calculated for photon energy less than 5 eV.

**Plasmon-induced structure in the optical interband absorption of free-electron like metals**, B. I. Lundqvist and C. Lydén, *SP323*, pp. 125-127 (Dec. 1971).

Key words: Electronic density of states; free-electron like metals; interband absorption; optical properties; plasmon; pseudopotential; quasi-particle; satellite structure.

We have extended Butcher's method to include the spectrum of interacting electrons, which contains satellite structure. The calculated optical conductivity shows a weak additional absorption, starting at about the frequency  $\omega_i + \omega_p$ , where  $\omega_i$  is the interband threshold frequency and  $\omega_p$  the plasma frequency.

**Theory of the photoelectric effect and its relation to the band structure of metals**, N. W. Ashcroft and W. L. Schaich, *SP323*, pp. 129-134 (Dec. 1971).

Key words: Electronic density of states; electron-electron scattering; electrons in a box; joint density of states; Kronig-Penney model; photoelectric effect.

We develop the theory of the external photoelectric effect in terms of quadratic response to the incident electromagnetic field. Electrons in the solid are in states determined by their interactions with themselves, the ions and the surface. We denote by  $H_0$  the Hamiltonian for this part. In the presence of the electromagnetic field we have a coupling term:

$$H_1 = -\frac{1}{c} \int d\mathbf{r} \mathbf{A}(\mathbf{r}, t) \cdot \mathbf{J}(\mathbf{r}) e^{i\eta}, \quad (\eta = 0^+)$$

where  $\mathbf{A}(\mathbf{r}, t)$  is the vector potential, and  $\mathbf{J}(\mathbf{r})$  is the current density operator for the electrons. Let  $\mathbf{R}$  be a point exterior to the solid. Then the expectation value of the operator measuring the external current density at  $\mathbf{R}$  in the states of  $(H_0 + H_1)$  is, to second order:

$$\langle J_\alpha(\mathbf{R}, t) \rangle = \left( \frac{1}{\hbar c} \right)^2 \int_{-\infty}^{\infty} d\tau_1 \theta(t - \tau_1) \int_{-\infty}^{\infty} d\tau_2 \theta(t - \tau_2) \cdot \sum_{\mu, \nu} \int d^3x_1 \int d^3x_2 A_\mu(\mathbf{x}_1, \tau_1) A_\nu(\mathbf{x}_2, \tau_2) \cdot \langle \langle J_\mu(\mathbf{x}_1, \tau_1) J_\alpha(\mathbf{R}, t) J_\nu(\mathbf{x}_2, \tau_2) \rangle \rangle.$$

There is no linear response and no other terms to order  $A^2$  giving a measurable result. We show that  $\langle J_\alpha(\mathbf{R}, t) \rangle$  may be related to the expectation value of the time ordered product of three current operators. This alternative description can be evaluated in the independent particle model (no scattering) and leads to a compact formulation of photoemission. There need not be a simple dependence of  $\langle J_\alpha(\mathbf{R}, t) \rangle$  or of its spectral reduction  $\langle J_\alpha(\mathbf{R}, t, e) \rangle$  (corresponding to measured electron distribution curves) on the joint density of states.

Rather  $\langle J_\alpha(\mathbf{R}, t, E) \rangle$  depends on the density of bound states but is not at all simply related to the density of states above the vacuum level. This emerges quite clearly from an analysis carried out in the well known constant matrix element approximation. A careful examination of the terms appearing in the photoelectric current shows that it is not always correct to interpret photoemission in terms of a "volume effect" or a "surface effect." The contributions from these two interfere. The usual explanations of the processes involved (i.e., the sequential operations of excitation, transport, and transmission) are also somewhat blurred.

The effect of electron-electron scattering is well known to be important and will be discussed both in terms of its manifestation in the observed electron distribution curves and its ability to limit the contribution of the conventional volume effect.

**Optical density of states ultraviolet photoelectric spectroscopy**, W. E. Spicer, *SP323*, pp. 139-157 (Dec. 1971).

Key words: Copper; copper nickel alloys; density of states; GaAs; Ge; nondirect transitions; optical density of states; PbTe; ultraviolet photoemission.

The use of ultraviolet photoemission to determine the density of valence and conduction states is reviewed. Two approaches are recognized. In one, the photoemission as well as other studies are used to locate experimentally a limited number of features of the band structure. Once these are fixed, band structure calculations could be carried out throughout the zone and checked against other features of the photoemission data. If the agreement is sufficiently good, the density of states is then calculated from the band structure. The second method depends only on experimental data. Using this approach, features of the density of states are determined directly by the photoemission experiment without recourse to band calculations. In cases where bands are wide and  $\mathbf{k}$  clearly provides an empirically important optical selection rule, this is possible only for portions of the bands which are relatively flat. Successful determinations of this type are cited for PbTe, and GaAs. In metals with narrow  $d$  bands such as Cu, it has been found empirically that one may explain fairly well the experimental energy distribution curves in terms of transitions between a density of initial and final states (the optical density of states, ODS) requiring only conservation of energy.

The ODS determined by such ultraviolet photoemission studies have more strong detailed structure than the density of states determined by any other experimental method. Studies on a large number of materials indicate that the position in energy of this structure correlates rather well with the position in energy of structure in the calculated density of states. It is suggested, following the very recent theoretical work of Doniach, that  $\mathbf{k}$  conservation becomes less important (and nondirect transitions more important) as the mass of the hole becomes larger. This is due to the change in  $\mathbf{k}$  of electrons in states near the Fermi level as they attempt to screen the hole left in the optical excitation process. These electrons take up the excess momentum. One would expect the  $\mathbf{k}$  conservation selection rule to play an increasingly important role as the mass of the hole decreases. This is in agreement with experiment.

**The density of states and photoemission from indium and aluminum**, R. Y. Koyama and W. E. Spicer, *SP323*, pp. 159-161 (Dec. 1971).

Key words: Aluminum (Al); direct and nondirect transitions; electronic density of states; indium (In); nondirect transitions; optical density-of-states; photoemission.



Experimental photoemission data from indium and aluminum are briefly described and can be understood in terms of a density of states model. In contrast to this, a direct transition model based on calculated band structures is found to yield photoelectron spectra which are fair reproductions of the density of states. This suggests that for these two metals, conclusions drawn concerning the density of states are independent of the model used to explain the photoemission data.

**Electronic densities of states from x-ray photoelectron spectroscopy,** C. S. Fadley and D. A. Shirley, *SP323*, pp. 163-178 (Dec. 1971).

**Key words:** CdCl<sub>2</sub>; density of states; HgO; noble metals; rigid band model; transition metals; x-ray photoemission; ZnS.

In x-ray photoelectron spectroscopy (XPS), a sample is exposed to low energy x rays (approximately 1 keV), and the resultant photoelectrons are analyzed with high precision for kinetic energy. After correction for inelastic scattering, the measured photoelectron spectrum should reflect the valence band density of states, as well as the binding energies of several core electronic levels. All features in this spectrum will be modulated by appropriate photoelectric cross sections, and there are several types of final-state effects which could complicate the interpretation further.

In comparison with ultraviolet photoelectron spectroscopy (UPS), XPS has the following advantages: (1) the effects of inelastic scattering are less pronounced and can be corrected for by using a core reference level, (2) core levels can also be used to monitor the chemical state of the sample, (3) the free electron states in the photoemission process do not introduce significant distortion of the photoelectron spectrum, and (4) the surface condition of the sample does not appear to be as critical as in UPS. XPS seems to be capable of giving a very good description of the general shape of the density-of-states function. A decided advantage of UPS at the present time, however, is approximately a fourfold higher resolution.

We have used XPS to study the densities of states of the metals Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Os, Ir, Pt, and Au, and also the compounds ZnS, CdCl<sub>2</sub>, and HgO. The *d* bands of these solids are observed to have systematic behavior with changes in atomic number, and to agree qualitatively with the results of theory and other experiments. A rigid band model is found to work reasonably well for Ir, Pt and Au. The *d* bands of Ag, Ir, Pt, Au and HgO are found to have a similar two-component shape.

**Direct-transition analysis of photoemission from palladium,** J. F. Janak, D. E. Eastman, and A. R. Williams, *SP323*, pp. 181-189 (Dec. 1971).

**Key words:** Copper; dielectric constant; direct interband transitions; electronic density of states; interband transition; Korringa-Kohn-Rostoker (KKR); "muffin-tin" potential; palladium (Pd); photoemission; plasmon; secondary emission; silver (Ag).

The energy distribution of optically excited electrons in Pd arising from direct interband transitions has been calculated assuming constant momentum matrix elements. Principal features of new photoemission data (*d*-band structure with four peaks at 0.15, 1.2, 2.2, and 3.5 eV below the Fermi level and a *d*-band width of ~ 3.8 eV) are successfully explained by these calculations. The data can be analyzed with comparable success using the nondirect-transition model, but only by assuming a free-electron density of unoccupied states, which is shown to be unjustified for Pd. In addition

to the photoemission spectra and the density of states, the imaginary part of the dielectric constant is computed and compared with experiment.

**Photoemission determination of the energy distribution of the joint density of states in copper,** N. V. Smith, *SP323*, pp. 191-197 (Dec. 1971).

**Key words:** Aluminum-insulator-palladium (Al-Pd); augmented plane wave method (APW); cesium; copper; direct transitions; electronic density of states; joint density of states; nondirect transitions; optical density of states; optical properties; photoemission.

Measurements have been made of the photoemission properties of cesiated copper, with improved sample preparation over the previous work by Berglund and Spicer. The energy distribution curves (EDCs) of photoemitted electrons show structure in the region associated with the copper *d* bands which was not seen in the previous data. The behavior in the photon energy range 6 to 8 eV is particularly interesting in that some of these new peaks in the EDCs are observed to move, appear and disappear in a manner characteristic of direct transitions.

Parallel calculations have been performed of the energy distribution of the joint density of states (EDJDOS) similar to those reported recently by Smith and Spicer. The band structure used was the interpolation scheme of Hodges, Ehrenreich, and Lang fitted to the APW calculation of Burdick. In a constant matrix element approximation, the EDJDOS represents the energy distribution of photoexcited electrons. This was converted to an energy distribution of photoemitted electrons by introducing appropriate threshold and escape factors. The overall agreement with experiment is good. In particular, some of the peaks in the theoretical EDCs are predicted to disappear and reappear on varying the photon energy, and there are strong similarities with the change observed experimentally.

It is found, therefore, that the optical transitions from parts of the copper *d* bands can be identified as direct. Theoretical calculations based on the EDJDOS work quite well for these and other transitions. Photoemission provides a very sensitive tool for verifying and even determining the EDJDOS. Burdick's bands for copper appear to be essentially correct over a wide range of energies including the whole of the *d*-band region, although minor modifications of a few tenths of an eV would improve agreement. It is found that the most persistent peaks in the calculated EDJDOS tend to coincide with the peaks in the calculated true density of states. This indicates that when a phenomenological "optical density of states" can be obtained, it may well be a good approximation to the true density of states even if transitions are direct.

**The band structure of tungsten as determined by ultraviolet photoelectric spectroscopy,** C. R. Zeisse, *SP323*, pp. 199-203 (Dec. 1971).

**Key words:** Carbon contamination; electronic density of states; photoemission; tungsten (W); UV photoemission; work function.

The technique of photoelectron spectroscopy has been used to probe the band structure of tungsten in the energy region where the *5d* bands are most prominent. The work function of the clean sample, a 25 micron thick polycrystalline foil, was found to be  $4.36 \pm 0.02$  eV, and the yield rose by three orders of magnitude from 5.0 to 11.3 eV without showing prominent structure of any other sort. The electron energy spectra, on the other hand, contain two pieces of reli-

able structure which are found to increase in energy at the same rate as the exciting photon energy. A simple analysis of the data gives evidence that the density of  $d$  states in tungsten consists of a shoulder just below the Fermi level, a peak located about 1.5 eV below the shoulder, and a broad peak which extends at least 7 eV below the Fermi level.

**Photoemission studies of scandium, titanium, and zirconium,** D. E. Eastman, *SP323*, pp. 205-208 (Dec. 1971).

**Key words:** Copper; direct versus nondirect transitions; electronic density of states; gold (Au); nondirect transitions; optical density-of-states; photoemission; scandium (Sc); silver (Ag); titanium (Ti); zirconium (Zr).

Photoemission spectroscopy studies of the hexagonal metals Sc, Ti and Zr in the 4 to 11.6 eV range have resolved  $d$ -band structure and have determined occupied  $d$ -band widths (at 1/2 maximum) of 1.6, 2.0 and 2.3 eV respectively. Resolved structure for all three metals correlates with structure in energy band density of states; however, the observed band widths for Ti and Zr are much narrower than previously calculated band widths. The relation of the data to the controversy concerning the nature of optical excitations in transition and noble metals (direct vs nondirect transitions) is discussed.

**Photoemission and reflectance studies of the electronic structure of molybdenum,** K. A. Kress and G. J. Lapeyre, *SP323*, pp. 209-215 (Dec. 1971).

**Key words:** Dielectric constant; electronic density of states; molybdenum (Mo); optical density of states; optical properties; photoemission; reflectivity; tungsten (W); zinc (Zn).

Normalized energy distributions of photoemitted electrons for  $4.3 < h\nu < 11.8$  eV (threshold is 4.3 eV) and near normal reflectance for  $0.5 < h\nu < 11.8$  eV are measured for molybdenum films prepared with ultra high vacuum. The nondirect transition model with constant matrix elements is found to be consistent with the photoemission data. The above model, in conjunction with calculations for the emission of scattered electrons, is used to obtain the optical density of states (ODS) for the occupied states. Three peaks due to  $d$ -electrons are observed at  $E - E_F = -0.5, -1.6$ , and  $-3.9$  eV where  $E_F$  is the Fermi energy. No structure is observed for  $E - E_F > 4.3$  eV. The imaginary part of the dielectric constant,  $\epsilon_2$ , is obtained by Kramers-Kronig analysis, and the occupied ODS are used to obtain the ODS for  $0 < E - E_F < 4.3$  eV. The latter analysis is done by writing the finite difference approximation for the integral expression of  $\epsilon_2$  and solving for the empty ODS. The ODS is compared to the band calculations of Mattheiss where a molybdenum density of states is obtained by scaling his tungsten (W) results. Both the measured and calculated occupied densities of states have three peaks and both empty states have one dominant peak. The calculations predict a low density of states for  $-1 < E - E_F < 0$  eV which is not observed in the data. The absorption coefficient has a minimum at 11.3 eV which correlates with a dip in the quantum yield. The energy distributions of the photoemitted electrons show small structural changes above the spectral range of the peak in the energy loss function at 10.8 eV. The relation of these data to the explanations based on the electron density of states for the anomalous isotopic mass dependence of the superconducting transition temperature is discussed.

**Ultraviolet and x-ray photoemission from europium and barium,** G. Brodén, S. B. M. Hagström, P. O. Hedén, and C. Norris, *SP323*, pp. 217-220 (Dec. 1971).

**Key words:** Barium (Ba);  $\beta$ -tungsten compounds; effects of oxidation; electronic density of states; europium (Eu); lanthanides; matrix elements; photoemission; rare-earth metals; UV and x-ray photoemission; x-ray photoemission.

Europium and barium are predicted to have very similar outer electronic structures with the exception that europium has a partially filled  $4f$  shell. Measurements are reported on photoemission from thin films excited with both vacuum ultraviolet and soft x-ray radiation. The results obtained using the low energy excitation indicate the similarity of the materials. Both show structure close to the leading edge in agreement with band structure calculations which indicate an increase in the density of states immediately below the Fermi level. Only a very small feature is observed with europium films which can be associated with the  $4f$  electrons. On the other hand using soft x-ray excitation a large peak corresponding to  $4f$  states lying 2.5 eV below the Fermi level is observed. The difference in the magnitudes is attributed to the size of the matrix elements involved.

**What is a quasi-particle?,** J. R. Schrieffer, *SP323*, pp. 227-231 (Dec. 1971).

**Key words:** Density of states; Green's function; mass enhancement; quasi-particle; superconductors.

The concept of a quasi-particle excitation in an interacting many-body system will be discussed from both the physical and the mathematical points of view. The physical origin of mass enhancement, wave function renormalization, interactions between quasi-particles, etc. will be presented. Landau's Fermi liquid theory, including the quasi-particle kinetic equation, will be reviewed. Finally, the domain of validity of the quasi-particle approximation will be discussed.

**Beyond the one-electron approximation: Density of states for interacting electrons,** L. Hedin, B. I. Lundqvist, and S. Lundqvist, *SP323*, pp. 233-247 (Dec. 1971).

**Key words:** Density of states; interacting electrons; one-particle Green function; oscillator strengths; quasi particle density of states; x-ray emission and absorption.

The concept "density of states" can be given many different meanings when we go beyond the one-electron approximation. In this survey we concentrate on the definition tied to excitation processes, where one electron is added or removed from the solid. We discuss the one-particle spectral function for conduction and core electrons in metals, how it can be approximately calculated, and how it can be related to different types of experiments like x-ray photoemission, x-ray emission and absorption, photoemission and optical absorption in the ultraviolet, and the Compton effect. We also discuss the form of the exchange-correlation potential for use in band structure calculations.

**Excitonic effects in x-ray transitions in metals,** G. D. Mahan, *SP323*, pp. 253-258 (Dec. 1971).

**Key words:** Density of states; exciton; many body effects; phase shifts; soft x-ray; transition probability.

In the study of soft x-ray transitions in solids, there has always been some hope that the results provide a direct measure of the density of states. This assumes that (a) matrix element variations over the band and (b) final state interactions are small. Both of these assumptions are known to be incorrect. To illustrate the possible strength of these effects, two approximate calculations are presented: the one electron oscillator strength of a simple bcc metal as a function of energy; and the strength of the Nozieres—DeDominicis sin-



gularity at threshold, with phase shifts estimated from an assumed Yukawa interaction between conduction electrons and core hole.

**Vibronic exciton density of states in some molecular crystals,** R. Kopelman and J. C. Laufer, *SP323*, pp. 261-267 (Dec. 1971).

Key words: Anthracene; aromatic crystals; benzene; excitonic density of states; molecular crystals; naphthalene.

Excited states of molecular crystals, which happen to be the majority of known crystals, are almost always classified as excitonic. The largest class of well studied systems are very closely described by the Frenkel model, and a majority of these systems can actually be described by a special case of the Frenkel model, one with steeply falling-off intersite (intermolecular) interactions. In this specific model the expression for the band structure depends only on the interchange symmetry of the crystal, with a small number of intersite parameters. Examples are given for some aromatic crystals, comparing band structures derived from theoretically calculated parameters, experimentally derived parameters, and completely experimentally derived band structure.

**Effect of the core hole on soft x-ray emission in metals,** L. Hedin and R. Sjöström, *SP323*, pp. 269-270 (Dec. 1971).

Key words: Aluminum; core hole; electronic density of states; Fermi edge singularity; pseudopotential; sodium (Na); soft x-ray emission.

We report a simple type of calculation to estimate the enhancement on the intensity of soft x-ray emission in free-electron like metals due to the effect of the core hole. We consider an electron gas in the presence of a perturbing potential and calculate the x-ray intensity assuming the dipole matrix elements to be constant. The calculation is based on a simple type of trial function for the initial state of the valence electron system and the coefficients are determined from the variation principle. The calculation does not give the Fermi edge singularity, which has recently aroused such a large interest, but instead aims at giving the gross effects for the whole spectrum. The results indicate an increase in the intensity by 25 to 50% at metallic densities. The enhancement factor is found to vary roughly linearly over the main band, increasing about 50% in going from the bottom of the band to the Fermi edge.

**Cancellation effects in the emission and absorption spectra of light metals,** B. Bergersen and F. Brouers, *SP323*, pp. 273-274 (Dec. 1971).

Key words: Electronic density of states; light metals; many-body effects; plasmon satellite; soft x-ray.

**Photoabsorption measurement of Li, Be, Na, Mg, and Al in the vicinity of K and  $L_{II,III}$  edges,** C. Kunz, R. Haensel, G. Keitel, P. Schreiber, and B. Sonntag, *SP323*, pp. 275-277 (Dec. 1971).

Key words: Aluminum (Al); beryllium (Be); electronic density of states; electron synchrotron light; K spectra; light metals; lithium (Li); L spectra; magnesium (Mg); photoabsorption; sodium (Na); transmission measurements.

The absorption structure of five light metals has been measured in the vicinity of the onset of K shell respectively  $L_{II,III}$  shell absorption. In accord with recent theoretical investigations a peaking of the cross section at the edge is observed for the  $L_{II,III}$  edges of Na, Mg, and less pronounced for Al. There is structure of a different type at the K edges of Li and Be.

**Optical absorption of solid krypton and xenon in the far ultraviolet,** C. Kunz, R. Haensel, G. Keitel, and P. Schreiber, *SP323*, p. 279 (Dec. 1971).

Key words: Electronic density of states; electron synchrotron light; krypton; optical absorption; xenon.

**The piezo soft x-ray effect,** R. H. Willens, *SP323*, pp. 281-285 (Dec. 1971).

Key words: Copper; electronic density of states; mechanical strain; modulation technique; nickel; soft x-ray.

In principle the soft x-ray emission spectrum should reveal the electronic structure of a material below the Fermi surface. In general, but for a few exceptions, the beginning and termination of the band structure are masked by low and high energy tails. The Van Hove singularities and critical points are unresolved due to effects such as Auger, lifetime and instrumental broadening.

The modulation of the  $L_{III}$  emission band of polycrystalline copper by an alternating elastic strain has recently been measured. Two effects are observed. First, there is an overall band shift which gives a measure of the deformation potentials. The band shift is not uniform as different subbands can shift varying degrees. For an applied load of 12,000 psi in uniaxial tension, the shift of the high energy side of the band is 0.015 eV and the low energy side is 0.010 eV. Because of the preferred orientation and polycrystalline nature of the sample, the exact microscopic sample is isotropic with a Young's modulus of  $20 \times 10^6$  psi, the average deformation potential is 25 eV at the top of the band and 17 eV at the bottom of the band. Secondly, superimposed on this band shift is structure which is unresolved in the normal emission spectrum. The origin of this structure is presumed to be from positions in the electronic structure which are extra sensitive to strain as far as altering the x-ray emission. This would be at Van Hove singularities or critical points where a high degree of degeneracy and wave function mixing is prevalent which can be changed by the symmetry alteration of the lattice due to strain. Comparison between the theoretical band structure calculations of copper and the emission structure due to strain modulation show several similarities.

The application of this technique to alloys should be useful for studying their electronic structure.

**Soft x-ray band spectra and their relationship to the density of states,** G. A. Rooke, *SP323*, pp. 287-293 (Dec. 1971).

Key words: Alloys; auger transitions; density of states; many-body interactions; plasmons; singularities; soft x rays.

The paper concentrates on the similarities and differences between the one-electron spectrum and the density of states; many-body effects, although important, are listed but they are not considered in detail. It is shown that the only reliable information about the density of states that can be obtained from soft x-ray spectroscopy are the energies of the Fermi surface and the van-Hove singularities, although the shape of the density of states can be derived indirectly from the energies of the van-Hove singularities.

It is the differences between the density of states and the one-electron spectra that may prove to be most important. These differences can give information about the symmetry and the local nature of the screening electrons. This is particularly interesting when studying alloys.

The Li K, the Al  $L_{23}$  and the Zn  $L_3$  spectra are given as examples which illustrate the above arguments. Finally, a brief discussion on the soft x-ray spectra from the Al-Mg system show how the results may be used to study alloys.



**Orbital symmetry contributions to electronic density of states of AuAl<sub>3</sub>**, A. C. Switendick, *SP323*, pp. 297-301 (Dec. 1971).

**Key words:** Augmented plane wave method (APW); electronic density of states; electronic specific heat; gold aluminide (AuAl<sub>3</sub>); "muffin-tin" potential; orbital density of states; soft x-ray emission.

From an augmented plane wave calculation of the valence and conduction bands of AuAl<sub>3</sub> we have constructed density of states histograms. From further calculations of the wave functions, one can attribute atomic-like character of the band states, e.g., Au 5*d*-bands, Al 3*s*-band, Al 3*p*-band. One can then partition the total density of states into atomic-like components according to the fractional atomic-like character of each state.

From the total density of states an electronic specific heat coefficient of 2.81 mJ/mole K<sup>2</sup> was calculated compared with the experimental value 3.03. The aluminum 3*s* density of states is compared with the aluminum L<sub>2,3</sub> soft x-ray emission spectra. Excellent agreement with experiment is obtained for the absolute location, and location relative to the Fermi energy, of the low energy peak. About half the calculated peak is attributable to tails of wave functions associated with the gold *d*-bands. Additional structure in the experimental curve is quite well reproduced in the calculation. This we take to be confirmation of the overall correctness of our bands.

**Soft x-ray emission spectrum of Al in AuAl<sub>3</sub>**, M. L. Williams, R. C. Dobbyn, J. R. Cuthill, and A. J. McAlister, *SP323*, pp. 303-305 (Dec. 1971).

**Key words:** Electron density of states; gold aluminide (AuAl<sub>3</sub>); gold-gallium (AuGa<sub>2</sub>); gold-indium (AuIn<sub>2</sub>); intermetallic compounds CsCl structure; L spectra; silver-aluminum alloys (AgAl); soft x-ray emission; *s*-orbital density of states.

Recently, Switendick and Narath have reported results of a systematic calculation of the electronic band structure of the compound series AuX<sub>2</sub> (X = Al, Ga, In). We have measured the L<sub>2,3</sub> soft x-ray emission spectrum of Al in AuAl<sub>3</sub> and from it, estimated the Al L<sub>3</sub> emission profile. We compare the latter to the distribution in energy of *s*-like charge at Al sites, estimated by Switendick from his band calculation. This *s* density is the dominant factor in a one-electron estimate of the soft x-ray emission rate. Quite good agreement is found, lending strong support to the calculations for AuAl<sub>3</sub>. This result also supports interpretation of a recently observed low energy peak in the L<sub>2,3</sub> emission spectrum of Al in Ag-Al alloys in terms of Ag *d* and Al *s-p* hybridization.

**Soft x-ray emission from alloys of aluminum with silver, copper, and zinc**, D. J. Fabian, G. Mc D. Lindsay, and L. M. Watson, *SP323*, pp. 307-312 (Dec. 1971).

**Key words:** Aluminum-copper alloys (AlCu); aluminum-zinc alloys (Al-Zn); electron density of states; silver aluminum alloys (Ag-Al); soft x-ray emission.

Measurements of the soft x-ray emission from the alloys Al-Ag, Al-Cu and Al-Zn are reported, and the effect of the *d*-bands of the metals Ag, Cu and Zn on the Al L<sub>2,3</sub>-emission for these alloys is examined. For Al-Ag and Al-Cu alloys, sharp resonance peaks are observed in the Al L<sub>2,3</sub>-spectra and are attributed to transitions from states in the hybridized silver and copper *d*-bands to core states of the aluminum atoms. The observations agree with the general theoretical considerations discussed by Harrison for a simple metal alloyed with a noble metal. For the Al-Zn alloys the *d*-bands of Zn do not contribute to the Al L<sub>2,3</sub>-emission.

**Soft x-ray emission spectra of Al-Mg alloys**, H. Neddermeyer, *SP323*, pp. 313-317 (Dec. 1971).

**Key words:** Aluminum (Al); aluminum-magnesium alloys (Al-Mg); charging effect; electronic density of states; emission spectra; magnesium (Mg); rigid-band approximation; soft x-ray emission.

In recent years the interpretation of soft x-ray emission band spectra has made good progress. With a detailed knowledge of the electronic band structure, of transition probabilities, and of lifetime broadening effects, it has been possible to calculate the shape of emission band spectra of a few pure elements. However, the situation is much more complicated in the case of alloys where the problems are far from being solved. The different shapes of emission band spectra of the components of an alloy make the applicability of the usual model to alloy spectra doubtful.

As a contribution to these problems we have remeasured the soft x-ray emission band spectra of Al-Mg alloys using improved experimental techniques. The Al L<sub>2,3</sub>- and Mg L<sub>2,3</sub>-emission spectra lying in the same wavelength region can be studied in the same spectrometer. Since the spectra of the pure metals have characteristic details and the energy resolution in this wavelength region is good, shapes and changes of shape can be registered very precisely.

**An L-series x-ray spectroscopic study of the valence bands in iron, cobalt, nickel, copper, and zinc**, S. Hanzely and R. J. Liefeld, *SP323*, pp. 319-326 (Dec. 1971).

**Key words:** Cobalt; copper; electronic density of states; iron; nickel; satellite emissions; self absorption; soft x-ray emission; x-ray spectroscopy; zinc (Zn).

This paper presents the results of an attempt to evaluate the merits of the soft x-ray spectroscopic method by examining a group of neighboring elements possessing a variety of valence band properties. The emission lines studied were the threshold level L<sub>α</sub> (valence → L<sub>III</sub> shell) lines obtained from high purity, polycrystalline bulk samples under bombardment by a nearly monoenergetic (ΔE ~ 1 eV) electron beam. The associated L<sub>III</sub> absorption spectra were obtained in this work as self-absorption curves from the same anode samples. Experimental and instrumental distortions were either eliminated, minimized or explicitly corrected for. The results indicate the presence of some anomalous emissions on the high energy side of the L<sub>α</sub> line in elements possessing a large density of unfilled valence levels just above the Fermi energy. The valence band emission line shape for these elements (iron, cobalt, and nickel) is found to be strongly dependent on the incident electron beam energy even for near-threshold-level excitations. Analysis of the emission and self-absorption curves demonstrates that the x-ray spectroscopic method is capable of exposing meaningful differences among the valence band energy structures of the solids examined here.

**The electronic properties of titanium interstitial and intermetallic compounds from soft x-ray spectroscopy**, J. E. Holliday, *SP323*, pp. 329-333 (Dec. 1971).

**Key words:** Electron concentration; electronic density of states; localized states; soft x ray; titanium compounds.

The TiL<sub>II,III</sub> emission bands (3*d* + 4*s* → 2*p* transition) have been obtained from TiC<sub>0.95</sub> and TiN<sub>x</sub> (x = 0.2 to 0.8) interstitial compounds and TiCr<sub>2</sub>, TiCo, TiNi and intermetallic compounds. Additional peaks on the low energy side of the TiL<sub>III</sub> band from TiC and TiN<sub>x</sub> appear to be cross transitions from the 2*s* and 2*p* bands of the nonmetal to the 2*p* level of titanium. Agreement was found between the soft x-

ray band spectra and the band calculations of Ern and Switendick on TiC and TiN. The soft x-ray emission spectra from TiC indicated strong admixture of the titanium 3*d* and carbon 2*p* bands which is in disagreement with LCAO band calculations of Lye and Logothetis. However, the 2*p* band of nitrogen was shown to be below the Ti 3*d* band indicating a localized state and a possible transfer of electrons from titanium to nitrogen.

The TiL<sub>III</sub> bands from TiCr<sub>2</sub>, TiCo and TiNi show a progressive change with increasing electronegativity difference between titanium and the combining element indicating possible ionic character to the bond. No peaks were observed in the low energy side of the TiL<sub>III</sub> bands, but a distinct splitting was observed in the peak of the TiL<sub>III</sub> band from TiNi.

**Soft x-ray emission spectrum and valence-band structure of silicon, and emission-band studies of germanium**, G. Wiech and E. Zöpf, *SP323*, pp. 335-337 (Dec. 1971).

Key words: Carbon; diamond; electronic density of states; germanium; kp method; orthogonalized plane wave (OPW) method; silicon; soft x-ray emission.

With a photon-counting concave grating spectrometer the L<sub>2,3</sub>-emission band of silicon and the energy range of the M<sub>2,3</sub>-emission band of germanium were investigated. The Si L spectrum shows new structural details. The measured intensity distribution for both the K- and L-emission bands of silicon are compared with recent calculations of the K- and L-emission spectra and with the density-of-states curve.

**Density of states in  $\alpha$  and  $\beta$  brass by positron annihilation**, W. Triftshäuser and A. T. Stewart, *SP323*, pp. 339-342 (Dec. 1971).

Key words: Angular correlation; brass; electronic density of states; positron annihilation.

Positron annihilation experiments using a long slit angular correlation apparatus have been performed to investigate the momentum distribution of photons resulting from positron annihilating with electrons in brass. Single crystals of  $\alpha$  and  $\beta$  brass which had been oriented along the 100, 110 and 111 directions respectively, were used for the measurements. The counter slits subtended an angle of 0.32 mrad at the sample. Thus, keeping the samples at liquid nitrogen temperature to reduce the positron motion, a total resolution of 0.42 mrad was achieved. The results show clearly deviations from a spherical Fermi surface. The observed anisotropies are found to agree very well with the theoretical predictions based on cross-sectional areas of the Fermi surface.

**Compton scattering from lithium and sodium**, P. Eisenberger and P. H. Schmidt, *SP323*, p. 345 (Dec. 1971).

Key words: Compton scattering; electronic linear momentum distribution function; lithium; potassium; sodium.

**Ion-neutralization spectroscopy**, H. D. Hagstrum, *SP323*, pp. 349-357 (Dec. 1971).

Key words: Auger processes; autoionization; density of states; ion-neutralization; transition probability.

The ion-neutralization spectroscopy (INS) is discussed in comparison with other spectroscopies of solids. It is shown that INS probes the local density of the solid at or just outside the solid surface. It is believed that this accounts for the clear-cut differences between INS results and those of other spectroscopies. Because of its unique specificity to the surface region INS is particularly useful in studying the surface

electronic structure of atomically clean surfaces and of surfaces having ordered arrays of known atoms adsorbed upon them. In the latter case INS determines a portion of the molecular orbital spectrum of surface molecules formed from the adsorbed foreign atom and surface atoms of the bulk crystal. Such spectra provide information on local bonding symmetry and structure and electrical charging within the surface molecule which is as yet unavailable by any other method. INS is the first attempt to base a spectroscopy of electronic states on a two-electron process. More recent work on experimental and mathematical problems which such a spectroscopy entails are also briefly mentioned in this paper.

**Potential and charge density near the interface of a transition metal**, E. Kennard and J. T. Waber, *SP323*, pp. 359-373 (Dec. 1971).

Key words: Absorption potential; charge density; metal-vacuum interface; platinum; surface energy.

The early literature on methods of calculating surface energy and charge density and of dealing with potential barriers at an interface are reviewed.

The three dimensional potentials and charge densities were obtained by superimposing the relevant atomic information which had been obtained from Dirac-Slater self-consistent field calculations on free atoms.

The total charge density at each point *P* was found by summing the contributions from atoms located within a sphere of radius *R* centered at *P*. The local exchange was estimated at *P* by means of Slater's  $\rho^{1/3}$  method. This was included with the overlapped atomic Coulomb potentials to obtain the crystal potential near the surface.

**Virtual impurity level density of states as investigated by resonance tunneling**, J. W. Gadzuk, E. W. Plummer, H. E. Clark, and R. D. Young, *SP323*, pp. 375-379 (Dec. 1971).

Key words: Anderson Hamiltonian; barium (Ba); calcium; chemisorption; electron density of states; field-emission resonance tunneling; germanium; tungsten (W); tunneling; zirconium.

The analogy between a virtual electronic state of an atom adsorbed on a metal surface and an Anderson type magnetic impurity state is pointed out. The density of states of the impurity can be characterized through a knowledge of the host induced shift and broadening of the atomic state. This density of states can be related to the current-voltage characteristics in a field-emission resonance tunneling experiment in the same manner as Appelbaum has done for describing spin flip Kondo type resonance tunneling in junctions.

Experimental current-voltage (field-emission total energy distribution) characteristics for single zirconium, barium, and calcium atoms on atomically perfect tungsten surfaces are analyzed in terms of the resonance tunneling theory described here and the virtual impurity level density of states is thus determined. Preliminary results for a metal-thin semiconductor-vacuum junction are also discussed.

**What properties should the density of states have in order that the system undergoes a phase transition?**, P. H. E. Meijer, *SP323*, pp. 381-384 (Dec. 1971).

Key words: Density of states; Ising model; Onsager model; partition function; phase transition; Weiss model.

We have solved nothing that needs to be solved regarding the density of states problem in a system that undergoes a phase transition. We, however, raise the question of what conditions the density of state function of the total system



(not the temperature dependent quasiparticle spectrum) should have in order that we are observing a phase transition. In general, one needs an extremely strong increase in the density—how strong can only be illustrated by using models. From these models we tried to obtain the density of states using the inverse Laplace transform. The results reveal that a vertical slope seems to be a necessary condition. There are reasons to believe that the condition is not sufficient.

**On deriving density of states information from chemical bond considerations,** F. L. Carter, *SP323*, pp. 385-405 (Dec. 1971).

**Key words:** Aromatic compounds; chemical bond; electronic density of states; Fermi surface; Pauling radii; transition metals; rare earth intermetallic compounds.

The chemical picture of bond formation between neighboring atoms in crystalline solids can give valuable electronic density of states information including the rough shape and relative filling of bands. In addition, from the representation of the chemical bond in momentum space one can readily predict the distortion of the Fermi surface from sphericity. This latter approach appears to provide an alternate explanation of the apparent attraction of the Fermi surface to the Brillouin zone faces.

The first relationship is best demonstrated in cases where relatively unique schemes of bond formation can be devised. This is possible in many intermetallic compounds having high coordination by the use of orthogonal sets of bidirectional orbitals; their use leads to multicenter bonds or cycles which are approximately orthogonal. Via the Fourier transform, the series of Slater determinants (representing the multicenter bond) can be transformed into momentum  $p$  space and then related to the usual band picture. The occupation or filling of bands can be estimated from bond orders of the associated bonds and obtained from known interatomic distances by using Pauling's metallic radii. Bond hybridization is obtained from orthogonality requirements and bond angle considerations characteristic of valence bond theory. These ideas can be applied to FCC and HCP transition metals. For copper one would expect a sharp peak in the density of states corresponding to two unshared filled local  $d$  orbitals. In addition there would be a broad bonding band filled with electrons (6 per atom) containing large amounts of  $p$  character; and a half-filled  $s$  band. As one moves downward through the periodic table to iron while maintaining either FCC or HCP structures the high melting points of the elements involved indicate that the broad bonding band remains relatively unchanged (filled) while the number of electrons in the narrow  $d$  band is steadily decreased.

In the rare earth cubic Laves phases of composition  $AB_2$ , this relatively simple chemical approach suggests the presence of four bands. The two more important bands are: (1) a large narrow-width density of states band associated with two unshared local  $d$  orbitals per B atoms, and (2) a band which is generally more than half-filled associated with all the transition metal B—B as well as the A—B bonds. The other bands include an  $s$  band associated with the B atoms which is less than half-filled due to the transfer of electrons from the hyper-electronic B atom, and a band of unusually high  $d$  character associated with the A—A bonds and probably not occupied for the lighter rare earth compounds.

From the study of simple  $\sigma$  bonds, Coulson has shown that the momentum distribution function is compressed in the direction of the internuclear axis. By using this idea in conjunction with the Fourier transform of hydrogenic atomic orbitals it is comparatively easy to show that for a

CCP transition metal like copper the momentum distribution function has its principal projections in the  $\langle 111 \rangle$  directions while the BCC transition metals should have projections in the  $\langle 110 \rangle$  directions. Projections in more complicated structures can be obtained from considerations of bond hybridization and bond order. In summary, we see that the valence bond concepts of bond hybridization and bond order coupled with known structures and bond distances can be used to suggest band shapes, filling, and hybridization. It is apparent that the increased use of chemical concepts in the interpretation of information concerning the electronic density of states is an area of promise.

**Electroreflectance observation of band population effects in InSb,** R. Glosser, B. O. Seraphin, and J. E. Fischer, *SP323*, pp. 407-410 (Dec. 1971).

**Key words:** Band population effects; electroreflectance; Fermi level shifts; indium antimonide (InSb); optical transitions; surface potential.

It is found that bias changes applied to  $n$ -InSb produce shifts in portions of the electroreflectance spectra. We attribute this to changes in the conduction band population produced as the separation between the Fermi level and the bottom of the conduction band is varied. Spectra which displays red, blue, or no shift correlates to electronic transitions starting from, ending at, or bridging the Fermi level. These observations permit a band structure identification of the shifting spectra and optical monitoring of the surface potential.

**Spin-orbit effects in the electroreflectance spectra of semiconductors,** B. J. Parsons and H. Piller, *SP323*, pp. 411-415 (Dec. 1971).

**Key words:** Critical points; diamond semiconductors; electroreflectance; gallium antimonide (GaSb); gallium arsenide (GaAs); germanium; semiconductors, diamond; semiconductors, zinc blende; spin-orbit splittings.

Measurements have been made of the electroreflectance spectra of germanium, gallium arsenide and gallium antimonide in the range of photon energies from 0.6 to 6.7 eV. Special attention has been paid to the resolution of multiplicity within the  $E_0'$  and  $E_1'$  structures. The identification of these structures in terms of critical point interband transitions involving the second conduction band has an important bearing on the band structure of these materials. The data is discussed in terms of the possible identification, within these higher energy multiplets, of spin-orbit splittings associated with the valence band states at  $\Gamma$  and L.

**Experimental verification of the predictions of the Franz-Keldysh theory as shown by the interference of light and heavy hole contributions to the electroreflectance spectrum of germanium,** P. Handler, S. Jasperson, and S. Koeppen, *SP323*, pp. 417-421 (Dec. 1971).

**Key words:** Electro-absorption techniques; electroreflectance; Franz-Keldysh theory; germanium; oscillatory dielectric function.

By the use of improved experimental techniques and samples of particular impurity concentration, we have been able to observe as many as eleven half oscillations in electroreflectance spectra of germanium at the direct edge ( $F_8^+ \rightarrow \Gamma_7^-$ ) at room temperature. In addition, near the experimental sixth half oscillation where the light and heavy hole contributions are of opposite signs, we observe destructive interference which greatly modifies the signal lineshape in that region. The unique characteristics of the resultant

lineshape allow the determination of the relative magnitudes of the dipole matrix elements and reduced masses for the two bands in a region of  $k$ -space somewhat removed from the  $\Gamma$ -point. The experimental results also demonstrate that neither thermal broadening nor field inhomogeneity need be a problem in electrodensity measurements.

**Variations of infrared cyclotron resonance and the density of states near the conduction band edge of InSb**, E. J. Johnson and D. H. Dickey, *SP323*, pp. 423-430 (Dec. 1971).

**Key words:** Cyclotron resonance; electronic density of states; electron-phonon interaction; InSb; interband transitions; Landau levels.

The electronic density of states near the conduction band edge of InSb with and without a magnetic field is obtained from dispersion relations based upon  $k \cdot p$  interactions with nearby bands and parameters determined and confirmed by several intraband experiments including fundamental cyclotron resonance, spin resonance, spin-flip cyclotron resonance, phonon assisted cyclotron resonance and harmonics of cyclotron resonance. The density of states displays effects due to nearby band interactions and due to electron-phonon interaction.

**Cyclotron resonances of holes in Ge at noncentral magnetic critical points**, J. C. Hensel and K. Suzuki, *SP323*, pp. 431-435 (Dec. 1971).

**Key words:** Cyclotron resonances; germanium; joint density of states; Landau levels; magnetic; magnetic critical points.

The anomalous, "quantum" cyclotron resonance spectrum of holes in the degenerate valence bands of Ge is analyzed utilizing the concept of a critical point in the magnetic joint density of states. Contrary to previous work done for  $k_H = 0$  (where  $k_H$  is the hole wave vector along the magnetic field) our results indicate that cyclotron resonance lines originating at critical points away from  $k_H = 0$  are responsible for most of the prominent features of the observed quantum spectrum in Ge.

**Landau level broadening in the magneto-optical density of states**, B. H. Sacks and B. Lax, *SP323*, pp. 437-450 (Dec. 1971).

**Key words:** Delta-function formulation of density of states; Green effect;  $k$ -conserving transitions; Landau levels; laser semiconductor; magneto-optical density of states; optical density of states; semiconductor laser.

In this paper we derive a convolution integral expression of the optical density of states for  $k$ -conserving transitions between broadened Landau levels in crystalline solids. The convolution is between single Landau level densities of states expressed in a form derived by Kubo. The expression includes as parameters the reduced mass, magnetic field strength, and the strength of the broadening mechanism. We present the results of numerical evaluation of this expression for various values of the parameters.

Our consideration is directed to dipolar transitions between the  $n=0$  Landau levels of the valence and conduction bands, and we assume that the dominant broadening effects are intraband scattering processes. This assumption is reasonable in view of the comparative intraband and interband lifetimes.

The resulting optical density of states function has an appearance identical to that of the single band function, but with the frequency measured from the gap energy replacing

the energy measured from the band edge, the reduced mass replacing the single band mass, and a reduced broadening parameter replacing the single band parameter. Our expression for this last parameter is shown to be a consequence of a mutual consistency requirement between the single band and optical densities of states, and this same requirement also leads to the reduced lifetime expression encountered in the more conventional Lorentzian formulation.

**The electronic structure of disordered alloys**, J. L. Beeby, *SP323*, pp. 453-463 (Dec. 1971).

**Key words:** Density of states; disordered alloys; one-electron propagator; perturbation expansion; sum rule.

The problem of calculating the electronic density of states in an alloy is considered from first principles. Choosing a suitably simplified model potential a diagrammatic expansion is discussed within which the various existing theories can be compared. Some comments are made on the comparison with experiment.

**Local theory of disordered systems**, W. H. Butler and W. Kohn, *SP323*, pp. 465-469 (Dec. 1971).

**Key words:** Binary alloys; density of states; disordered systems; periodically continued neighborhood.

The most striking characteristic of crystalline solids is their periodicity. As a result of this feature, theoretical descriptions of physical phenomena in such systems are usually given in wave number or momentum space. The reciprocal lattice of a crystal and the Fermi surface of a metal are examples. In a disordered system, on the other hand, there is no such periodicity and momentum space descriptions are much less natural. However, in such systems, physical conditions near a point  $r$ , in coordinate space, become independent of the conditions at a distant point  $r'$ , provided that  $|r-r'|$  is large compared to either a characteristic mean free path or some other appropriate length. This suggests that one can analyze a macroscopic disordered system by averaging over the properties of microscopic neighborhoods.

In the present paper we report some details of such a program. Although the point of view is of quite general applicability we have, for the sake of definiteness, studied so far only one type of system: Noninteracting electrons moving in the field of interacting, disordered scattering centers. We have focused especially on the electronic density of states. The macroscopic system is represented by an average over small neighborhoods. If one did not take special precautions, one would encounter one class of errors of the order of  $d/L$  where  $L$  is a characteristic dimension of the neighborhood, and  $d$  is a characteristic atomic dimension; and another class of errors of the order of  $1/N$  where  $N$  is the number of ions. Both are too large to be tolerable for practical purposes. However, by an appropriate treatment of the statistical mechanics of the scatterers and by periodic repetition of the small neighborhoods, these errors can be avoided. The remaining errors are exponentially small in the ratio  $\gamma(L/R)$  where  $\gamma$  is of order unity and  $R$  is the smaller of the electronic mean free path or the deBroglie wavelength of the electrons. This exponential convergence of the small neighborhood theory promises to make it a useful practical method for the study of disordered systems, especially very highly disordered ones.

Numerical examples are presented and discussed.

**Density of electron levels for small particles**, L. N. Cooper and S. Hu, *SP323*, pp. 473-475 (Dec. 1971).

**Key words:** Diffusion equation; electronic density of



states; "muffin-tin" potential; small particles; two dimensional classical membrane.

The density of electronic levels for small particles is calculated. This differs from the usual expression which is valid as the volume of the sample becomes very large. The leading term of the correction is proportional to the surface/volume of the sample. Depending on the environment the density of electronic levels may be increased or decreased.

**One-dimensional relativistic theory of impurity states**, M. Steślicka, S. G. Davison, and A. G. Brown, *SP323*, pp. 477-480 (Dec. 1971).

Key words: Impurity states; Kronig-Penney model; one-dimensional Dirac equation.

The one-dimensional Dirac equation is solved for the Kronig-Penney model containing a  $\delta$ -potential impurity. Depending on certain existence conditions, the impurity states can be classified into two types called relativistic and Dirac impurity states. In the nonrelativistic limit, the Dirac states disappear and the relativistic ones become the ordinary impurity states. A detailed discussion is given of the complete energy spectrum.

**The influence of generalized order-disorder on the electron states in five classes of compound-forming binary alloy systems**, E. W. Collings, J. E. Enderby, and J. C. Ho, *SP323*, pp. 483-492 (Dec. 1971).

Key words: Binary alloys;  $\text{Bi}_2\text{Te}_3$ ;  $\text{CdSb}$ ; copper-gold ( $\text{Cu-Au}$ );  $\text{Cu}_3\text{Au}$ ;  $\text{CuPt}$ ;  $\text{Cu}_3\text{Pt}$ ; ductility; electrical resistivity; Hall effect; magnesium bismide ( $\text{Mg}_3\text{Bi}_2$ ); mechanical behavior; melting; model potential of Heine and Abarenkov; nickel aluminide; order-disorder; Peierls barriers; Pt-Cu; silver<sub>2</sub> tellurium ( $\text{Ag}_2\text{Te}$ ); Ti-Al; TiCo; TiFe; TiNi;  $\text{Ti}_2\text{Te}$ .

The influence of generalized order-disorder (including solid-state order-disorder, and melting) on electronic structures will be discussed for various types of binary intermetallic compounds which, for the purpose of discussion, will be arbitrarily subdivided into five classes. Classes A and B exhibit solid-state order-disorder (O-D) reactions. In the first of these the atomic potentials are sufficiently similar that the use of low-order perturbation theory at all concentrations is valid. The effect of O-D on such alloys will be described in relationship to the density-of-states, as measured by low-temperature specific heat and magnetic susceptibility, and to the electrical transport properties, particularly the conductivity and Hall coefficient. We then consider from the same standpoint a second type of system in which the potentials are sufficiently different as to produce bound states which appear in the *ordered* form. The disappearance of these bound states when the alloy disorders gives rise to characteristic electronic behavior.

The effect of O-D on the experimental parameters referred to above will be compared for the two types of systems. In particular, published data for Cu-Au, as a representative example of the first type of system, will be contrasted with new electronic property data for Ti-Al, and compared with recent experimental results for Pt-Cu, which occupies an intermediate position. In class C, which is metallic in the solid, and in classes D and E which are semiconducting in the solid, structural order persists up to the melting point. For D the liquid is metallic, and data are presented for  $\text{Bi}_2\text{Te}_3$ , a typical system of this class. The conditions for the existence of intermetallics of class E are extreme, and give rise to nonmetallic behavior in the liquid.

These various systems will be discussed in terms of differences in atomic potentials. The major problems involved

in giving precise estimates of the required differences will be outlined and a critical account of the use of concepts like the electronegativity parameter will be presented.

**Localized states in narrow band and amorphous semiconductors**, D. Adler and J. Feinleib, *SP323*, pp. 493-503 (Dec. 1971).

Key words: Amorphous semiconductors; Anderson transition; augmented plane wave method (APW); chalcogenide glasses; electronic density of states; Franck-Condon principle; localized states; Mott insulator; NiO; optical density-of-states; photoconductivity; photoemission; polaron.

The electronic density-of-states is discussed in situations where some of the states near the Fermi energy are localized, due to either intraionic Coulomb repulsion or disorder. When localized states are present, the Franck-Condon principle necessitates separate electrical and optical densities-of-states. In the case of ionic Mott insulators, it is shown that doping or nonstoichiometry drastically affects the energy-band structure. For the particular example of NiO, introduction of  $\text{Li}^+$  impurities or excess oxygen leads to a large upward displacement of the  $2p$  band associated with the oxygen ions, moving it sufficiently near the Fermi level that hole conduction in the  $2p$  band predominates above 200 K, in agreement with the available experimental data. In the case of amorphous semiconductors, it is shown that introduction of electron-electron and electron-phonon interactions results in a shift of the relative position of the localized parts of the valence and conduction bands, as well as shifts of the localized states relative to the itinerant states. However, the qualitative features of the model of Cohen et al. are preserved.

**A cluster theory of the electronic structure of disordered systems**, K. F. Freed and M. H. Cohen, *SP323*, pp. 505-507 (Dec. 1971).

Key words: Amorphous semiconductors; band tail of localized states; cluster theory; coherent potential approximation; disorder systems; electronic structure; Neel temperature.

The equation of motion for the averaged Green's function in an alloy couples the latter to the Green's function for which the average is restricted so that the composition of one atom is held fixed. The average Green's function may be regarded as the Green's function for a zero-atom cluster, and it is coupled to the Green's function for a one-atom cluster. There is thus an infinite hierarchy of equations of motion in which the  $n$ -atom functions are coupled to the  $(n+1)$ -atom functions. The coherent potential approximation of Soven corresponds to truncation in the equation of motion of the one-atom function. We have generalized the coherent potential theory to a theory the  $n$ -atom functions with truncation in the equation of motion of the  $(n+1)$ -atom function. The formalism is developed and a few of the results obtained thus far are presented in this paper.

**T matrix theory of density of states in disordered alloys—application to beta brass**, M. M. Pant and S. K. Joshi, *SP323*, pp. 509-514 (Dec. 1971).

Key words: Alloys; brass; delta-function potential; disordered systems; Green's functions; Korringa-Kohn Rostoker (KKR); "muffin-tin" potential; short-range-order parameters; spectral density of states;  $t$ -matrices.

The  $T$  matrix theory of electronic states in disordered systems, has been used to determine the spectral density for states of various symmetries, for binary alloys. Soven's

averaged  $t$  matrix procedure is improved by retaining the distinction between the  $t$  matrices of the constituents, and introducing partial Greenians of the Pant-Joshi theory. Information about the pair-correlation function obtained by critical neutron scattering method is used to evaluate the partial Greenians, as well as the crystalline potentials for the constituents. In order to facilitate computation of the  $t$  matrices, these potentials have been replaced by energy-dependent model potentials. The parameters of the model potentials are determined by the requirement that they yield logarithmic derivatives (of the radial wave function at the muffin-tin spheres) identical with those generated by the real potentials. The scheme has been applied to disordered beta-brass. The separation in energy of the peaks of the spectral density of states at the high symmetry points of the Brillouin zone, are compared with experimental results, and with the results obtained by the virtual crystal approximation.

**On the terms excluded in the multiple-scattering series**, R. M. More, *SP323*, pp. 515-518 (Dec. 1971).

**Key words:** Delta-function potential; excluded terms; Green's functions; multiple-scattering series; rigid-band approximation; scattering phase-shifts;  $t$ -matrices.

We have evaluated certain of the excluded terms in the multiple-scattering series for a simple soluble potential. We discuss three aspects of the result: first, the reduction to "on-shell" quantities; second, the numerical contribution of the excluded terms; and third, the analytic properties of these terms.

**On non-localization at the centre of a disordered bound band**, F. Brouers, *SP323*, pp. 521-526 (Dec. 1971).

**Key words:** Cellular disorder; disordered systems; electronic density of states; localization life-time; quasi-localized state; tight-binding.

It is shown for a three dimensional model of tightly bound electrons with cellular disorder that the electronic states at the middle of a continuous band cannot be strictly localized. This conclusion is just the opposite of what has often been suggested.

Nevertheless, an approximate calculation of the electron localization "life-time" suggests that with increasing disorder the localized character of the electron states become more pronounced.

It is argued that in such a system there is no sharp transition between localized and non-localized regions of the energy spectrum.

**The half-filled narrow energy band**, L. G. Caron and G. Kemeny, *SP323*, pp. 527-541 (Dec. 1971).

**Key words:** Antiferromagnetic insulator; first order phase transition; half-filled narrow energy band; Mott state; paramagnetic metal;  $t$ -matrix.

The antiferromagnetic and paramagnetic states of a half-filled narrow energy band are investigated using a  $t$ -matrix approach. This method is justified despite the high particle density in the system. A phase diagram including the Mott state is given. Employing the gap of the antiferromagnetic insulator as a variational parameter, it is shown that the increase of the band width potential energy ratio leads to a first order phase transition into the paramagnetic metal state, nearly where Mott has estimated it to occur.

**Electronic structure of gold and its changes on alloying**, E. Erlbach and D. Beaglehole, *SP323*, pp. 545-549 (Dec. 1971).

**Key words:** Electronic constant; electronic density of

states; gold (Au); gold-copper alloys (Au-Cu); gold-iron alloys (Au-Fe); gold-silver alloys (Au-Ag); optical constants; reflectivity.

We have measured the changes in reflectivity upon alloying small amounts of Ag, Cu and Fe into Au. By means of a Kramers-Kronig analysis, we have deduced the changes in  $\epsilon_2$  produced by this alloying. We relate these changes to shifts in the position and character of the electron energy bands in gold.

**Density of states of AgAu, AgPd, and AgIn alloys studied by means of the photoemission technique**, P. O. Nilsson, *SP323*, pp. 551-554 (Dec. 1971).

**Key words:** Coherent potential approximation; electronic density of states; Friedel screening theory; photoemission; silver-gold alloys (AgAu); silver-indium alloys (AgIn); silver-palladium alloys (AgPd); virtual crystal approximation.

The density of states of AgAu, AgPd, and AgIn alloys have been studied by means of the photoemission technique. General trends of the results are compared with the predictions from simple models of alloys. The rigid-band or virtual-crystal approximation cannot explain the results, while model calculations in the coherent potential approximation reproduces the observed density of states. The Friedel screening theory explains the shift of the Fermi level on alloying.

**Density of states information from low temperature specific heat measurements**, P. A. Beck and H. Claus, *SP323*, pp. 557-562 (Dec. 1971).

**Key words:** Alloys; density of states; low temperature specific heat; magnetic specific heat; many-body effects; superconductivity.

The calculation of one-electron density of state values from the coefficient  $\gamma$  of the term of the low temperature specific heat linear in temperature is complicated by many-body effects. In particular, the electron-phonon interaction may enhance the measured  $\gamma$  as much as twofold. The enhancement factor can be evaluated in the case of superconducting metals and alloys. In the presence of magnetic moments, additional complications arise. A magnetic contribution to the measured  $\gamma$  was identified in the case of dilute alloys and also of concentrated alloys where parasitic antiferromagnetism is superimposed on an over-all ferromagnetic order. No method has as yet been devised to evaluate this magnetic part of  $\gamma$ . The separation of the temperature-linear term of the specific heat may itself be complicated by the appearance of a specific heat anomaly due to magnetic clusters in superparamagnetic or weakly ferromagnetic alloys.

**Electronic density of states determined by electronic specific heat measurements**, T. Mamiya and Y. Masuda, *SP323*, pp. 565-568 (Dec. 1971).

**Key words:** Augmented plane wave method (APW); Debye temperatures; electronic density of states; electron-phonon coupling constant; electronic specific heat; superconducting transition temperatures; tantalum (Ta); tantalum-rhenium (Ta-Re) alloys; Ta-Re alloys.

The superconducting transition temperatures, electronic specific heats, and Debye temperatures have been recently measured by us for  $5d$  transition-metal alloy series Ta-Re. By making use of these data and the theoretical predictions by McMillan, we have deduced the electron-phonon coupling constant and bare electronic density of states. The



density of states is compared with the theoretical one derived from band-structure calculations of Ta using the augmented-plane-wave (APW) method by Mattheiss.

**Low-temperature specific heats of hexagonal close-packed erbium-thulium alloys**, A. V. S. Satya and C. T. Wei, *SP323*, pp. 571-577 (Dec. 1971).

**Key words:** Anti-ferromagnet; anti-phase domain; augmented plane wave method (APW); Curie temperature; electronic density of states; enhancement factors; erbium; erbium-thulium alloys; ferro-magnetic spiral structure; gadolinium; itinerant 4f-band model; lanthanides; low-temperature specific heat; rare-earth lanthanides; specific heats; spin-wave theory; thulium.

The specific heats of hexagonal close-packed erbium and thulium metals, and three of their isostructural alloys were measured in the liquid-helium temperature range between 1.3 and 4.2 K for examining the validity of the localized 4f-band model, on which the current theories of the rare-earth metals are based. Barring possible uncertainties in the magnetic properties of the samples and their impurity contents, the coefficients of the specific-heat component linear in temperature calculated from the present data range in values approximately two to twenty times the constant electronic specific-heat coefficient predicted by the above model for all the hexagonal close-packed rare-earth lanthanides. Possible explanations for such discrepancies are discussed. An itinerant 4f-band model based on the one-electron-band model suggested by Mott is proposed for the lanthanides as an alternative to the localized 4f-band model.

**Low-temperature specific heats of face-centered cubic Ru-Rh and Rh-Pd alloys**, P. J. M. Tsang and C. T. Wei, *SP323*, pp. 579-585 (Dec. 1971).

**Key words:** Electronic density of states; electronic specific heat; palladium (Pd); Rh; Rh-Pd alloys; Ru-Rh alloys; specific heat; tight-binding approximation.

The specific heats of Rh, Pd, and a number of face-centered cubic Ru-Rh and Rh-Pd alloys were determined between approximately 1.4 and 4.2 K. Whereas the  $C/T$  vs.  $T^2$  plots for the Ru-Rh alloys show a straight-line behavior, a low temperature anomaly is observed in similar plots for Pd and the Rh-Pd alloys below 2.2 K. This low temperature anomaly appears to be most pronounced in the alloy  $Rh_{0.78}Pd_{0.22}$ , and diminishes with increasing Rh or Pd. The electronic specific heats of these alloys are generally high with a minimum occurring at  $Ru_{0.30}Rh_{0.70}$ . A portion of the total density-of-states curve for the outer electronics in face-centered cubic transition metals is derived numerically from the present results and those available in the literature as a first approximation. Such a curve shows qualitative agreement with the first peak below Fermi level of the theoretical total  $s$ - $d$  density of Pd calculated by Janak et al.

**Density of states of transition metal binary alloys in the electron-to-atom ratio range 4.0 to 6.0**, E. W. Collings and J. C. Ho, *SP323*, pp. 587-596 (Dec. 1971).

**Key words:** Alloys; bcc transition metal alloys; charging effect; electronic density of states; Ginzburg-Landau coherence length; G.P. zone; Hf-Ta; low-temperature specific heat; magnetic susceptibility; omega phase; rigid-band approximation; superconducting transition temperatures; tantalum-tungsten (Ta-W); Ti-Mo; titanium-molybdenum (Ti-Mo) alloy; tungsten (W); W-Re.

Using Ti-Mo as a prototype of binary bcc transition metal alloys for  $4 < e/a < 6$ , densities-of-states at the Fermi level,

$n(E_F)$ , have been studied using low-temperature specific heat augmented by magnetic susceptibility ( $\chi$ ) measurements. A survey of the literature has revealed that the principal descriptors of density of states,  $\gamma$  (the electronic specific heat coefficient), and  $T_c$  (the superconducting critical temperature), generally decrease as  $e/a$  decreases below about  $e/a \sim 4.3$  to 4.5. The maxima in  $\gamma$  and  $T_c$  so induced have usually been interpreted as indicating the existence of maxima in  $n(E_F)$  near  $e/a \cong 4.5$  for bcc alloys. But since the region  $e/a \lesssim 4.5$  also corresponds to that in which a sub-microscopic hexagonal-structured precipitate ( $\omega$ -phase) always appears in quenched alloys, a detailed study of microstructure was undertaken in conjunction with the electronic property measurements. It was concluded that a steadily increasing abundance of an  $\omega$ -phase precipitate was responsible for the observed drops in  $\gamma$ ,  $T_c$ , and  $\chi$  below  $e/a \cong 4.5$ . Because of the fineness of the precipitate (70-330 Å) the physical property results themselves are indistinguishable from those usually associated with single-phase materials. Using magnetic susceptibility at elevated temperatures, where the prototype Ti-Mo alloy is known to be single phase bcc, it has been shown that  $n(E_F)_{bcc}$  increases monotonically as  $e/a$  is reduced from 6 to 4, in agreement with deductions based on the results of recent band-structure calculations on bcc 3d transition metals.

**Specific heat of vanadium carbide, 1-20 K**, D. H. Lowndes, Jr., L. Finegold, D. W. Bloom, and R. G. Lye, *SP323*, p. 597 (Dec. 1971).

**Key words:** Electronic density of states; specific heat vanadium carbide.

**Relevance of Knight shift measurements to the electronic density of states**, L. H. Bennett, R. E. Watson, and G. C. Carter, *SP323*, pp. 601-642 (Dec. 1971).

**Key words:** Electronic density of states; hyperfine fields; Knight shift; nuclear magnetic resonance; susceptibility; wave functions.

The Knight shift,  $\mathcal{K}$ , measures the magnetic hyperfine field at the nucleus produced by the conduction electrons which are polarized in a magnetic field. Knight shifts are often dominated by the Pauli term and, in its most simple form, can be written as  $\mathcal{K} = \langle a \rangle \chi_p$ . Here  $\chi_p$  is the conduction electron Pauli spin susceptibility which depends on the density of states at the Fermi level,  $N(E_F)$ , and  $\langle a \rangle$  is an average magnetic hyperfine coupling constant associated with the wave function character at the nucleus,  $|\psi_F(0)|^2$ , for conduction electrons at the Fermi surface.

The Knight shift therefore provides, through  $\langle a \rangle$ , insight into the wave-function character associated with  $N(E_F)$ . Calculations of  $\langle a \rangle$  involving an averaging over  $k$ -space have been attempted for a few simple metals up to the present time. For alloys and intermetallic compounds, rather different  $\langle a \rangle$ 's are experimentally observed for different local environments, indicating that  $\mathcal{K}$  samples the variation in local wave-function character, or a variation in local density of states. There is no unique way of separating the local variation of  $N(E_F)$  from  $|\psi_F(0)|^2$ .

In this article the methods developed for relating  $\mathcal{K}$  to the electronic properties for most of the types of cases encountered in the literature are reviewed. We discuss "simple" metals including problems of orbital magnetism and changes in  $\mathcal{K}$  caused by electronic transitions such as melting. Knight shifts and their temperature dependence in metals and intermetallic compounds involving unfilled  $d$  shells, are discussed. We give estimates of atomic hyperfine fields due to single electrons, appropriate to those cases where

problems due to electronic configurations do not make deductions from experiment too ambiguous. A density of states curve calculated for Cu is given, showing the relative importance of *s*-*p*, and *d* character for that metal. In a qualitative sense this Cu curve implies such information for other transition metals. We discuss alloy solid solutions for the cases where a "rigid" band model might be used to explain the results, and for cases where local effects have to be taken into account. The charge oscillation and RKKY approaches and their limitations are reviewed for cases of dilute nonmagnetic and *d*- or *f*-type impurities.

**Pauli paramagnetism in metals with high densities of states**, S. Foner, *SP323*, p. 645 (Dec. 1971).

**Calculation of the Knight shift in beryllium**, J. Gerstner and P. H. Cutler, *SP323*, p. 649 (Dec. 1971).

**Key words:** Beryllium; Knight shift; orthogonalized plane wave (OPW); pseudopotential.

**Knight shifts of the alkali metals**, A. Meyer, G. M. Stocks, and W. H. Young, *SP323*, pp. 651-657 (Dec. 1971).

**Key words:** Alkali metals; alloys; cesium; Knight shift; lithium; potassium; pressure dependences; pseudopotential; resistivity ratios; rubidium; sodium; thermoelement power.

K, Rb and Cs, being leading members of transition series, have pseudoatoms with virtual bound *d* states; Li has a somewhat analogous *p* state. By contrast, Na has no such states. Evidence is offered of how the associated scattering accounts for the following observed electron transport properties: (a) Under pressure, the resistance of Li rises and, eventually, so do those of Cs, Rb and K, (b) the thermopower of Li is anomalous (positive) and stays so under pressure while that for Cs very quickly becomes positive when pressure is applied.

The same features can now be used in the theory of Knight shifts to explain the following observations. (c) The conduction electron susceptibility for Li is enhanced very significantly above that for free (and even interacting) electrons, (d) the nuclear contact density in Li is much lower than that predicted by one-OPW theory, (e) the Knight shifts of Li and Na decrease and those for Rb and Cs increase when pressure is applied, (f) the Knight shift for a given ion increases when it is successively resonated in Na, K, Rb, and Cs matrices. The key to the interpretation of (e) and (f) is the variation in the density of states (and therefore susceptibility) under conditions of pressure change and alloying.

**Role of exchange effects on the relationship between spin susceptibility and density of states of divalent metals**, P. Jena, T. P. Das, S. D. Mahanti, and G. D. Gaspari, *SP323*, pp. 659-662 (Dec. 1971).

**Key words:** Be; Cd; density of states; divalent metals; exchange enhancement; Mg; spin susceptibility.

The influence of exchange and correlation of conduction electrons on the spin susceptibility,  $\chi_s$ , is well understood in alkali metals. There is reasonable agreement between theoretical and experimental results where the latter are available. No such comparison has been reported for the divalent metals, mainly because of a lack of experimental information. Only for Be is  $\chi_s$  known (from spin resonance measurements). We have made semi-empirical estimates of  $\chi_s$  for Mg and Cd by adjusting the measured Knight shifts with theoretical values of the core polarization and  $\langle \psi^2(0) \rangle$ . The values of  $\chi_s$  so deduced are compared to theoretical estimates made by the method of Silverstein, who treated

the exchange enhancement by an interpolation procedure analogous to that of Nozières and Pines for calculating correlation energies, and included the effects of band structure through the calculated thermal (band) effective mass. Agreement is good for Mg, which behaves more like a free electron metal, and poor for Be and Cd. Possible sources of the discrepancies are discussed.

**Correlation of changes in Knight shift and soft x-ray emission edge height upon alloying**, L. H. Bennett, A. J. McAlister, J. R. Cuthill, and R. C. Dobbyn, *SP323*, pp. 665-670 (Dec. 1971).

**Key words:** Aluminum oxide ( $\text{Al}_2\text{O}_3$ ); electronic density of states; gold aluminide ( $\text{AuAl}_2$ ); Knight shift; magnesium-aluminum alloy phases; nickel aluminide ( $\text{NiAl}$ ); soft x-ray emission.

In simple metals and alloys—those having no significant local *d*-character at or near the Fermi level—the Knight shift provides a measure of the local *s*-electron density of states. If the particular atom under study has a *p*-like core level, then soft x-ray emission arising from transitions of electrons at the Fermi level into *p*-like core vacancies should provide a similar measure. Using Al as the example, we compare results of these two techniques by studying fractional changes, relative to Al metal, of the Knight shift and  $L_{2,3}$  soft x-ray emission edge height of Al in  $\text{NiAl}$ ,  $\text{AuAl}_2$ ,  $\text{Mg}_2\text{Al}_3$ ,  $\text{Mg}_{17}\text{Al}_{12}$ , and  $\text{Al}_2\text{O}_3$ . A distinct correlation is observed.

**Tunneling measurements of superconducting quasi-particle density of states and calculation of phonon spectra**, J. M. Rowell, *SP323*, pp. 673-679 (Dec. 1971).

**Key words:** Density of states; phonons; semiconductors; superconductivity; tunneling.

It is an unfortunate fact that the tunneling technique, which has proved incredibly successful in the study of superconductivity, has given little information about the normal state properties of metals and semiconductors. It will be shown that, in the determination of the superconducting quasi-particle density of states, it is the change in density induced by the onset of superconductivity which is measured rather than the total density.

Returning to the problem of normal materials, a review of the limited achievements and failures of tunneling will be presented. This will include the influence of band edges on tunneling in *p-n* diodes and metal-semiconductor contacts, the structures observed in tunneling into bismuth and the negative results obtained in nickel and palladium. The dominant effect of the change in barrier shape in most of these tunneling characteristics will be illustrated.

**Density of states from superconducting critical field measurements**, G. Dummer and D. E. Mapother, *SP323*, pp. 681-684 (Dec. 1971).

**Key words:** Critical field; density of states; In; pressure dependence; superconductivity; Tl.

For a superconducting metal, the entropy difference,  $\Delta S$ , between the normal and superconducting states is thermodynamically related to the critical field,  $H_c$ , by the equation

$$\Delta S = S_n - S_s = 1 (VH_c/4\pi) (dH_c/dT),$$

where  $V$  is the molar volume and  $T$  is the absolute temperature. As the temperature approaches 0 K, it can be shown that  $\Delta S$  is dominated by the normal electronic entropy,  $\gamma T$ , where  $\gamma$  is the temperature coefficient of the normal electronic specific heat. This behavior has been known for a long time but its application has been largely confined to in-



ferences based on conjectural extrapolations of  $H_c$  data measured about 1 K. In the limit of very low temperatures where  $\Delta S = \gamma T$ , it follows that

$$H_c^2(T) = H_0^2 - (4\pi\gamma/V)T^2,$$

where  $H_0$  is the limiting value of  $H_c$  at 0 K. For most superconductors the range of validity of this expression lies below 1 K but new techniques have made this range relatively accessible in recent years. Within this range precise static measurements of  $H_c$  and  $T$  permit determination of the ratio,  $\gamma^* = (\gamma/V)$ , with a relative accuracy of about 1:3000. This is considerably better than the accuracies typically obtained in low temperature calorimetry. This method has been used to study the change in  $\gamma^*$  under hydrostatic pressures up to 1000 atm for In and Tl. Nonlinear changes in  $\gamma^*$  are clearly resolved for the first time, despite the relatively low values of applied pressure. For In the values of  $\gamma^*$  show a parabolic decrease with increasing pressure. The results for Tl show an initial increase in  $\gamma^*$  which reaches a maximum near  $p = 500$  atm. For larger pressures the value of  $\gamma^*$  shows the normal decrease with increasing  $p$ .

**Temperature dependence in transport phenomena and electronic density of states for transition metals**, M. Shimizu, *SP323*, pp. 685-690 (Dec. 1971).

Key words: Chromium; electronic density of states; iridium; low-temperature specific heat; magnetic susceptibility; molybdenum; niobium; palladium (Pd); platinum; rhenium; rhodium; rigid band approximation; tantalum (Ta); thermal conductivity; thermoelectric power; transition metal; transport properties; tungsten (W).

The calculated results of the temperature variations of electronic specific heat and spin susceptibility and their comparison with the experimental results for various transition metals are briefly summarized. In these calculations the empirical densities of states, which were determined in the rigid band model from the experimental data of low temperature specific heat coefficient, were made use of. In a model similar to the Mott model of  $s$ - $d$  scattering, the electrical resistivity, thermal conductivity, and thermoelectric power have been calculated at high temperatures for palladium, platinum, rhodium, iridium, molybdenum, and tungsten, by assuming appropriate electronic structures and making use of the same empirical densities of states. The calculated temperature dependences of electrical resistivity, thermal conductivity, and thermoelectric power and the sign of the thermoelectric power at high temperatures are found to be strongly dependent on the shape of the density of states and the position of the Fermi level. It is shown that all of these temperature dependences and the sign of the thermoelectric power are consistent with the experimental results. It is confirmed that there is a strong correlation between these temperature dependences and those of the electronic specific heat and spin susceptibility.

**Metal-semiconductor barrier junction tunneling study of the heavily doped  $n$ -type silicon density of states function**, Y. Hsia and T. F. Tao, *SP323*, pp. 693-712 (Dec. 1971).

Key words: Antimony-doped silicon; arsenic-doped silicon (As doped Si); band absorption; band tailing; depletion layer barrier tunneling; electronic density of states; Esaki diode; gallium-arsenide (GaAs); heavy doping with As, Ga, P, Sb; luminescence experiments; P doped Si; Schottky-barrier; silicon; transport properties; tunneling.

Experimental and analytic techniques and procedure used in the study are described. Experimental data showing the

dependency of the Fermi level on the dopant types of the heavily doped  $n$ -type silicon are reported. A dopant type dependent density of states effective mass is postulated to describe the effect of different dopants on the Fermi level. The deviation of the experimental data curve from the calculated curve is ascribed to the effect of degenerate semiconductor band tailing. In addition, through interpretation of incremental conductance versus applied bias characteristic curves of the different tunnel junction evaluated, a consistent description of the density of states function of the heavily doped silicon is obtained. The density of states function, dependent on the dopant type and dopant concentration, is generally parabolic above the band edge, but towards the band edge, band tailing can be severe.

**The effect of hydrostatic pressure on the galvanomagnetic properties of graphite**, I. L. Spain, *SP323*, pp. 717-725 (Dec. 1971).

Key words: Electronic density of states; galvanomagnetic properties; graphite; Hall Effect; magneto-resistance; pressure effects.

Measurements of the Hall Effect and magneto-resistance in crystals of graphite with current flow in the basal planes at high pressures are described. Galvano-magnetic measurements enable the magneto conductivity tensor components  $\sigma_{xx}$  and  $\sigma_{xy}$  to be obtained, and from them the electron and hole densities and mobilities. The results are compared with the band model for the semi-metal graphite proposed by Slonczewski and Weiss. Of particular interest at the present time is the information that these results give about the assignment of carriers at the symmetry point  $K$  in the Brillouin zone of graphite and the properties of mobile minority carriers.

**Electrical resistivity as a function of hydrogen concentration in a series of palladium-gold alloys**, A. J. Maeland, *SP323*, pp. 727-729 (Dec. 1971).

Key words: Electron donation model; electronic density of states; gold-palladium alloys; hydrogen absorption; hydrogen in palladium-gold alloys; palladium-gold alloys; rigid-band approximation.

The changes occurring in the electrical resistance of a series of gold-palladium alloys during hydrogen absorption have been measured. The results are presented for each alloy in the form of relative resistance,  $R/R_0$  vs. hydrogen concentration  $H/M$ ;  $R$  is the resistance of a particular gold-palladium alloy containing a certain amount of hydrogen, given by  $H/M$ , the atomic ratio of hydrogen to metal, and  $R_0$  is the resistance of the same *hydrogen free* alloy. For pure palladium the relative resistance increases as a function of hydrogen concentration to a maximum value of  $\sim 1.80$  at  $H/M \approx 0.75$ ; further hydrogen absorption results in a decrease in  $R/R_0$ . Similar maxima are found in some gold-palladium alloys; however, the maxima occurs at decreasing  $R/R_0$  values and also shifts to lower  $H/M$  values with increasing gold concentrations. At sufficiently high gold contents the maximum disappears and a continuous decrease in resistance with increasing hydrogen content occurs. The results are evaluated in terms of the band model.

**The volume dependence of the electronic density of states in superconductors**, R. I. Boughton, J. L. Olsen, and C. Palmy, *SP323*, pp. 731-734 (Dec. 1971).

Key words: Aluminum (Al); electronic density of states; electronic specific heat; gallium; Gruneisen parameter, electronic; superconductivity; thermal expansion; thorium; volume dependence of density-of-states.

The volume dependence of the electronic specific heat coefficient  $\gamma$  can be obtained from measurements of the low temperature thermal expansion, from observations on the pressure dependence of the superconducting threshold curve, and from the volume change occurring at transition. We make use of recent theoretical results to obtain values of the change in the density of states with volume from the existing experimental data for a number of metals.

**Alloy Fermi surface topology information from superconductivity measurements**, H. D. Kaehn and R. J. Higgins, *SP323*, pp. 735-736 (Dec. 1971).

**Key words:** Electronic density of states; Fermi surface; In-Cd alloys; pressure; strain; superconductivity.

**Hydrogenation effects on palladium tunnel junctions**, W. N. Grant, R. C. Barker, and A. Yelon, *SP323*, pp. 737-739 (Dec. 1971).

**Key words:** Al-oxide-Pd; electronic density of states; hydrogen in palladium; rigid-band approximation; tunnel junctions.

The effects of hydrogenation on the electron tunneling characteristics of Al-oxide-Pd junctions have been investigated. It is found that the impedance of the junctions increases from 1 to 5 percent with increasing hydrogenation, with the greatest increase occurring at large positive bias on the Pd. We attribute this effect to the introduction of electrons from hydrogen into the  $d$  bands of palladium.

**Calculation of thermodynamic information based on the density of states curves of two allotropes of iron**, D. Koskimaki and J. T. Waber, *SP323*, pp. 741-752 (Dec. 1971).

**Key words:** Electronic density of states; iron; phase transitions; thermodynamic information.

The use of density of states curves to obtain thermodynamic information associated with the allotropic phase transitions in iron is discussed. The density of states curves for both body-centered cubic and face-centered cubic iron are determined using a program which randomly interpolates between previously calculated eigenvalues to generate a large number of new energy solutions. These new eigenvalues enable a more accurate determination of density of states curves than is possible by plotting and averaging the original eigenvalues themselves. The density of states curves determined for each phase are used to obtain the energy sum of the eigenvalues of the valence electrons, the shift in the Fermi potential with temperature for the two curves, and the electronic specific heat versus temperature curves for both phases of iron over the temperature range from 0 K to the melting point.

**Potential-independent features of crystal band-structure**, M. M. Saffren, *SP323*, p. 755 (Dec. 1971).

**Key words:** Band structure; crystal potential; electronic density of states; pseudopotential.

**Nonlinear optical susceptibility of semiconductors with zincblende structure**, M. I. Bell, *SP323*, pp. 757-766 (Dec. 1971).

**Key words:** Electronic density of states; gallium arsenide (GaAs); indium antimony (InSb); indium arsenide (InAs); joint density of states; nonlinear optical susceptibility; optical properties; semiconductors; zincblende structure; ZnTe.

A simple model for the band structure and electronic density of states in zincblende semiconductors has been used to calculate the dispersion of the nonlinear susceptibility responsible for second-harmonic generation. The calculation

requires no adjustable parameters, and results have been obtained for GaAs, InAs, ZnTe, and InSb in substantial agreement with experiment in the energy range 0-2.0 eV.

**Model density of states for high transition temperatures beta-tungsten superconductors**, R. W. Cohen, G. D. Cody, and L. J. Vieland, *SP323*, pp. 767-773 (Dec. 1971).

**Key words:** Beta-tungsten; lattice transformation; model electronic density of states; superconductivity.

We have applied a simple density of states model to the problem of superconductivity in high  $T_c$  beta-tungsten superconductors. If we assume that the interaction responsible for superconductivity is predominately between  $d$ -band carriers and acoustic phonons via a deformation potential matrix element, simple analytic expressions for the effective electron-electron coupling constant  $\lambda$  and  $T_c(\lambda)$  can be obtained. The quantities  $\lambda$  and  $T_c$  can then be estimated using parameters determined from an application of the density of states model to the cubic state constants. We are able to establish the simple condition  $\lambda > \lambda_{crit} \approx 0.7$  for the existence of a cubic-tetragonal lattice transformation in these materials. Using our result for  $T_c$ , we find  $T_c \geq 15$  K for all materials which exhibit a lattice transformation. Thus, we have established the relation between high  $T_c$  superconductivity and lattice transformation in the  $\beta$ -W compounds.

**Summary of the conference on electronic density of states**, H. Ehrenreich, *SP323*, pp. 775-781 (Dec. 1971).

**Thermal electron effective mass of rubidium and cesium**, D. L. Martin, *SP323*, p. 783 (Dec. 1971).

**Key words:** Cesium; effective mass; electronic density of states; rubidium; specific heat.

**Density of states and numbers of carriers from the dHvA effect**, S. Hornfeldt, J. B. Ketterson, and L. R. Windmiller, *SP323*, pp. 785-790 (Dec. 1971).

**Key words:** Electronic density of states; de Haas van Alphen effect; Fermi surface; Fermi velocity; Fourier series; spherical harmonics; symmetrized techniques.

With the dHvA effect, one can determine the angular dependence of the extremal area and effective mass over all sheets of the Fermi surface. Using recently developed techniques this data can be inverted and the angular dependence of the Fermi radius and Fermi velocity determined. Techniques have been developed to allow the inversion of both open and closed surfaces. For closed surfaces we use an expansion in symmetry adapted spherical harmonics (to order  $l=60$ ) while for open surfaces a three-dimensional Fourier series representation is used. With this information one may determine, for a given sheet of the surface, the number of carriers  $n(E_F)$  and density of states  $N(E_F)$  by performing the appropriate integrations.

**A note on the position of the "gold 5d bands" in AuAl<sub>2</sub> and AuGa<sub>2</sub>**, P. D. Chan and D. A. Shirley, *SP323*, pp. 791-793 (Dec. 1971).

**Key words:** Electronic density of states; gold aluminum two (AuAl<sub>2</sub>); gold gallium two (AuGa<sub>2</sub>); x-ray photoelectron spectroscopy.

Switendick and Narath recently proposed a solution for the "AuGa<sub>2</sub> dilemma" pointed out by Jaccarino et al. This solution was based on the results of band structure calculations. The density of states for AuAl<sub>2</sub> derived from these band-structure calculations were presented at this conference.



ference. A surprising result of this calculation was the position of the "gold  $d$ -band" states. These states were located at about  $-7$  eV in AuAl<sub>2</sub> and at similar energies in AuGa<sub>2</sub> and AuIn<sub>2</sub>. The interesting optical properties of gold intermetallic compounds (e.g., AuAl<sub>2</sub> is violet) are often attributed to the proximity of the gold  $d$ -bands to the Fermi energy,  $E_F$ . If these states really lay at  $E_F-7$  eV, and were as flat (i.e., the  $\rho(E)$  peak was as narrow) as the calculation indicated, then they could scarcely affect the compounds' optical properties. To help resolve this " $d$ -band dilemma," we undertook measurements of the valence-band spectra of AuAl<sub>2</sub> and AuGa<sub>2</sub> by x-ray photoelectron spectroscopy (XPS). This method has been described elsewhere; accordingly we describe below only those experimental features of this work that were peculiar to the AuAl<sub>2</sub>-AuGa<sub>2</sub> problem. The two compounds are first treated in separate sections. The results are then discussed in the final section.

**The reliability of estimating density of states curves from energy band calculations**, E. B. Kennard, D. Koskimaki, J. T. Waber, and F. M. Mueller, *SP323*, pp. 795-800 (Dec. 1971).

Key words: Aluminum; electronic density of states; free electron parabola; QUAD scheme; reliability of smoothing procedures.

The density of states curve for aluminum was calculated for different initial energy bands using the quadratic interpolation method (QUAD) developed by Mueller et al. In one case, a true parabolic energy band was used as input and in the second, the  $E(k)$  values were those obtained for aluminum by Snow using the APW method. Deviations from the parabolic density of states curve were found to be inversely proportional to the number of  $E(k)$  values per histogram box and hence inversely proportional to the square root of the number of  $k$  points in the Brillouin zone. It was necessary to use 100,000 points to obtain a relative deviation of 0.3%. In the second case, the self consistent band calculations for 2048 points in the full Brillouin zone and for a subset of 256 of these were used as input data. The effect of increasing the number of input values was assessed for 25,000 random points in the Brillouin zone. The relative errors were 26 and 9 respectively for 256 and 2048 points.

The effects of "smoothing" as an alternative method of reducing statistical error in computing density of states curves are also discussed.

**SP329. Supplement 1. An index of U.S. voluntary engineering standards**, W. J. Slattery, Editor, Nat. Bur. Stand. (U.S.), Spec. Publ. 329, Suppl. 1, 459 pages (Dec. 1972).

Key words: Engineering Standards, index of; index of standards, recommended practices, specifications, test methods; Key-Word-In-Context index of voluntary standards; standards, voluntary, index of.

This supplement contains the permuted titles of more than 6,300 standards, specifications, test methods, and recommended practices published by 225 U.S. technical societies, professional organizations and trade associations. Each title can be found under all the significant key words which it contains. These key words are arranged alphabetically down the center of each page together with their surrounding context. The date of publication or last revision, the standard number and an acronym designating the standards-issuing organization appear as part of each entry.

**SP330, 1972 Edition. The international system of units (SI)**, C. H. Page and P. Vigoureux, Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 330, 45 pages (Apr. 1972).

Key words: General Conference of Weights and Measures; International Committee of Weights and Measures; Interna-

tional System of Units; SI; Système International des Unités; Units of Measurement.

This translation from the French "Le Système International d'Unités, (SI)" published originally by the International Bureau of Weights and Measures (BIPM) has been prepared jointly by the National Physical Laboratory, UK, and the National Bureau of Standards, USA. Included are Resolutions and Recommendations of the General Conference of Weights and Measures (CGPM) on the International System of Units, together with relevant extracts from the International Organization for Standardization (ISO) for the practical use of the system.

Appendix I gives in chronological order the decisions promulgated since 1889 by CGPM and the International Committee of Weights and Measures (CIPM) on units of measurement and on SI. Appendix II outlines the measurements, consistent with the theoretical definitions given in this document which metrological laboratories can make to realize the units and to calibrate precision material standards. Appendix III describes the laboratory and the committees which come under the Metre Convention. (Supersedes NBS Special Publication 330, 1971 Edition.)

**SP348. The science of ceramic machining and surface finishing.**

Proceedings of a symposium sponsored by the American Ceramic Society, the Office of Naval Research, and the National Bureau of Standards, Nov. 2-4, 1970, held at NBS, Gaithersburg, Md., S. J. Schneider, Jr., and R. W. Rice, Editors, and C. F. Bersch, A. M. Diness, and J. B. Wachtman, Jr., Associate Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 348, 431 pages (May 1972).

Key words: Ceramic machining; ceramics; mechanical effects of machining; removal and shaping of ceramics; surface treatment.

This volume presents the proceedings of the Symposium on the Science of Ceramic Machining and Surface Finishing held at the National Bureau of Standards in Gaithersburg, Md., on Nov. 2-4, 1970. The symposium was jointly sponsored by the Baltimore-Washington Section of the American Ceramic Society, the Office of Naval Research, and the National Bureau of Standards. The purpose of the conference was to survey the developing science of ceramic machining and to stimulate further progress by discussion of current problems and research programs. In addition to a panel discussion, 37 review and original research papers were presented with attention focused on four main areas: (1) Techniques and Mechanisms of Removal and Shaping (2) Surface Treatment (3) Analysis and Characterization of Machining Effects and (4) Mechanical and Other Effects of Finishing. An edited version of the floor discussion following each paper is given. *These proceedings include the following papers (indented):*

**Science and the machining and surface finishing of ceramics**, R. W. Rice, C. F. Bersch, and A. M. Diness, *SP348*, pp. 1-3 (May 1972).

Key words: Machining; machining costs; methods of machining and finishing; surface-dependent properties; surface finishing.

Historically, the technology of machining and surface finishing of ceramics has advanced by empirical methods. Further advances appear limited without gaining basic knowledge of the mechanisms of removing or redistributing material from or on ceramic surfaces. Because of the diversity of ceramic behavior, this is a challenging scientific problem. However, meeting this challenge can result not only in improved or new machining and finishing processes, but also in greater understanding of the character of the resultant surface and sub-surface, and hence of the surface-dependent properties.

Mechanical methods of ceramic finishing, P. J. Gielisse and J. Stanislaw, *SP348*, pp. 5-35 (May 1972).

Key words: Abrasive; ceramics; diamond; fracture; grinding; grinding forces; grinding temperatures; machining; polishing; residual stresses; stock removal; surface analysis; theory of grinding.

Mechanical methods of finishing ceramics have been reviewed based on current practice as well as past and present research results. A total systems evaluation involves technical process and economic parameters. State of the art information indicates a need for scientific evaluation of the basic stock removal process.

Experiments simulating grinding with single point diamond tools have generated quantitative and qualitative data on mechanical, dynamic, and thermal aspects of the stock removal process. Generation of the data involved specially designed techniques.

Analysis of the results have been made in terms of mechanical, geometric, and material parameters. A mechanical and thermodynamic model is presented.

Direct observation of material removal process during grinding of ceramics by micro-flash technique, O. Imanaka, S. Fujino, and S. Mineta, *SP348*, pp. 37-43 (May 1972).

Key words: Alumina; brittle fracture; chip removal process; forsterite; glass-ceramics; grinding of ceramics; micro-flash technique; observation of chips during grinding; steatite.

In order to make the mechanism of grinding ceramics clear, chip removal processes have been observed during grinding with a specially-built setup which consists of a flash lamp, synchronizer, microscope, and motor-driven camera. Duration time of the flash is about  $0.8 \mu\text{s}$  in half-value width, and a storage capacitor in the flash lamp circuit can store an energy of about  $10 \text{ W} \cdot \text{s}$ . By choosing the flashing point, grinding phenomena at different positions on the contact arc can be photographed at certain time intervals.

The experiments were done mainly by using one grain of diamond attached to a disk which was mounted on a shaft of a surface grinding machine. Workpiece materials examined were glass-ceramics and several types of oxide ceramics, e.g., alumina, forsterite, and steatite ceramics. The main results obtained are as follows: Under moderately large depth of cut, the chips generated from ceramics are generally of a fragment type and are distinguished from those of ductile materials. Part of these chips were observed to be removed, of course, directly by the grain, but a considerable part of them were found to splinter out of the workpiece surface in a short time after the grain has passed over. Possible explanations are proposed for those phenomena. The above-mentioned facts suggest that a damaged layer may remain under the ground surface of ceramic materials. It is also demonstrated that chips of continuous type are occasionally observed at high grinding speed and under moderately small depth of cut. The chip formation of this type depends delicately on the materials to be ground.

Grinding—A means of shaping and sizing ceramics, J. A. Mueller, *SP348*, pp. 45-52 (May 1972).

Key words: Capability; ceramics; grinding wheels; selection; shaping; sizing.

The shaping and sizing of ceramic bodies can be done with abrasive grinding wheels. From a grinding wheel point of view, ceramic bodies may be classified into two groups.

One group that is harder than 800 Knoop and the other group that is softer than 800 Knoop.

The materials that are harder than 800 Knoop generally require the use of diamond wheels. Diamond wheels have the capability to remove stock, to generate precise geometry, and to produce finishes as fine as those that are measured in light bands.

The selection of the diamond grinding wheel is critical because improper selection can cause excessive grinding costs, poor quality, and low productivity. The selection of the diamond grinding wheel includes not only the selection of the specification of the wheel formulation but also the selection of the geometry of the wheel.

Case histories of finishing and shaping ceramic bodies illustrate the capability of the grinding wheel in these areas. Suggestions for starting speeds, feeds, and wheels together with a list of practical everyday "Rules of Thumb" for efficient grinding are documented.

Aspects of machining glass-ceramic materials, G. H. Allgeyer and L. V. Colwell, *SP348*, pp. 53-57 (May 1972).

Key words: Abrasive machining; brittle chip formation; brittle fracture; chip accommodation; glass; glass-ceramics; machining and grinding technical ceramics; material removal rate; specific energy; wheel structure.

The manufacture of optical and mechanical parts from glass-ceramic materials usually requires the removal of unwanted stock resulting from casting, hot forming, or the cutting of blocks from large ingots or blanks. Desired surface finishes at specified dimensions are the usual requirements. Conventional metalworking cutting tools did not produce satisfactory results. Scratching, splintering, and brittle fracture were responsible for the material removal action in the sawing, drilling, turning, and milling operations attempted. Very rough unsatisfactory surfaces resulted.

The physical and mechanical properties of CER-VIT® material classify it as a brittle, crystalline material in the usual machining state. The best controllable means of material removal was found to be abrasive machining. The high hardness (550 Knoop) and abrasive character of these materials conclusively recommend diamond as the most satisfactory cutting medium. Machinability studies were conducted on CER-VIT® glass-ceramic material using diamond abrasive tooling while adjusting the controllable machining variables. The results and relationships of these techniques as applied to CER-VIT® glass-ceramic are discussed.

Significance of the experimental results is explored with particular emphasis being placed upon the predictable performance of diamond tools and the feasibility of programming of machining variables for utilization of numerically controlled machining processes.

The principles of grinding, R. S. Hahn and R. P. Lindsay, *SP348*, pp. 59-71 (May 1972).

Key words: Abrasive wear parameter; grinding; material removal parameter; principles of grinding; surface finish in grinding; surface integrity in ground surfaces; wheel dressing.

Three distinct actions are shown to take place in the grinding process, namely rubbing, ploughing, and cutting. A clue to the relative importance of each of these can be obtained by plotting the volumetric rate of stock removal against the wheel/work interface force for unit width (force intensity). Such plots show for some materials a threshold force intensity below which no stock removal occurs. Equations relating the stock removal rate and the interface force



intensity are developed and a "material removal parameter" is defined. Similar equations for the wheel wear and a "wheel-wear parameter" are also developed. It is found for many materials that the stock removal rate is a linear function of the interface force intensity. However, the abrasive removal rate or dimensional wheel wear is found to vary approximately as the square of the interface force intensity. Increasing wheel surface speed is generally found to raise the material removal parameter.

The essential parameters in dressing with single pointed diamonds are introduced and their effect on controlling the sharpness of a grinding wheel is discussed. Semi-empirical equations for predicting wheel wear are given in terms of force intensity, wheel hardness, and wheel-workpiece conformity. The factors influencing surface finish are described, including the dressing lead, the depth of cut of the dresser diamond, and the interface force intensity. Thermal damage and surface integrity are discussed. The existence of a threshold force intensity (or feed rate) below which no thermal cracking takes place is shown. Raising the workspeed tends to raise this threshold. Wheel sharpness is also found to be an important variable, and means for quantitatively measuring wheel sharpness are given.

**A basic study of the diamond grinding of alumina, D. M. Busch and J. F. Prins, *SP348*, pp. 73-87 (May 1972).**

**Key words:** Abrasion; chatter vibrations; forces in grinding; fracture of alumina grains; grinding noise; grinding of alumina; scratching of glass; single diamond cutting of alumina.

Experiments were performed using single diamond points to cut Coors AD96 alumina under conditions simulating the grinding of this material. These studies involved different diamond particles and the forces were recorded during the cutting action.

Parallel to the single diamond experiments, grinding tests were performed on the same ceramic material using the same types of diamonds with which the single point studies were done. The grinding experiments and the single diamond experiments were then compared to get a better understanding of the actual cutting mechanism involved when grinding aluminium oxide.

The wear of the diamond particles and the damage inflicted on the ceramic material were studied with the aid of electron microscopy. A relationship was found between the forces measured, the deterioration of the bonding material, and the wear of the diamonds.

Special attention was given to diamonds of the MDA-S type, a blocky, sharp-edged diamond grit, and diamond spheres. These two types of diamonds were compared in grinding and showed similar results due to the production of flat areas on the spheres and the movement and wear of the blocky particles in the bonding material to present flat faces to the workpieces.

The grinding experiments also entailed a study of machine vibrations, especially chatter vibrations and the grinding noise associated with it.

**On the strength of ceramics as a function of microstructure, grinding parameters, surface finish, and environmental conditions, R. Sedlacek, F. A. Halden, and P. J. Jorgensen, *SP348*, pp. 89-96 (May 1972).**

**Key words:** Alumina; delayed fracture; grinding of ceramics; microstructure; stress corrosion; vacuum strength.

The tensile strength of four aluminas is described in terms of their microstructure and composition. The effect of microstructure on the attainable surface finish is discussed,

and the results of profilometric evaluation of ground surfaces are presented. Various postgrind treatments are shown to have differing effects on microstructure. Griffith's flaw theory is applied to aluminas of different grain sizes, and calculated strengths are found to agree with experimental data. The phenomena of delayed fracture and stress corrosion are discussed; the strength of alumina is found to be higher under vacuum than in air and is independent of stress rate.

**Grinding alumina with diamond abrasives, R. J. Caveney and N. W. Thiel, *SP348*, pp. 99-112 (May 1972).**

**Key words:** Alumina; cylindrical grinding; diamond grinding wheel; electron microscopy; removal mechanism; surface damage; surface finish; surface grinding; wear mechanism.

This paper is the result of a preliminary investigation into the grinding of high density alumina with diamond abrasive grinding wheels.

Following extensive work on the application of diamond for tungsten carbide and steel grinding, the De Beers Diamond Research Laboratory recently embarked on a research programme to study the various aspects of ceramic grinding. In the Diamond Abrasive Technology Centre's Grinding Section, ceramics with three different alumina contents were ground with a variety of diamond types both natural and synthetic to establish what effect changes in wheel speed have when surface grinding these materials. The mode and extent of damage of the ground surfaces of the specimens were investigated using conventional electron microscopy. In addition to these investigations, measurements were made of the quality of the surface finishes that can be obtained under different grinding conditions. Variations in grinding efficiency, machining costs, and surface damage are discussed for the three alumina grades tested. The mechanism of wear of the different diamond types was studied and is demonstrated by means of scanning electron micrographs.

Also reported in this paper are the initial results obtained from tests on cylinders of the same three alumina grades mentioned above. These initial tests were aimed at finding the most suitable combination from the point of view of wheel life, of wheel and workpiece speeds, and incorporated tests with both natural and synthetic grits.

**Ceramic substrate and specimen fabrication, H. C. Leistner and W. A. Wilson, *SP348*, pp. 113-117 (May 1972).**

**Key words:** Ceramics; finishing; grinding; specimens; substrates; ultrasonic machining.

Procedures have been developed to fabricate ceramic materials used as substrates for precision, coaxial, thin film resistors. Excellent radio frequency characteristics have been obtained from this procedure in developing radio frequency standards at the National Bureau of Standards at power levels of 10 milliwatts to 100 watts and frequencies from direct current to 4.0 gigahertz. Substrates fabricated for this purpose require precise tolerances and surface finish to insure uniformity of thin films deposited on a ceramic substrate.

In addition, procedures have been developed to fabricate specimens used in determining the dielectric and magnetic properties of ferrites, insulating ceramics, glass, fused silica, and single crystal materials. A variety of shapes are required including spheres, rods, disks, and ellipsoids. Precise tolerances are required to obtain qualitative property measurements of the materials involved.

In both procedures, special techniques are used with existing equipment in grinding ultrasonic machining, lapping, and polishing to obtain the required end product. This paper deals with both the application of the required products and the methods used to fabricate these products.

**On the shaping of brittle solids by erosion and ultrasonic cutting,** H. L. Oh, K. P. L. Oh, S. Vaidyanathan, and I. Finnie, *SP348*, pp. 119-131 (May 1972).

**Key words:** Abrasion; brittle-ductile transition; erosion; fracture location; ring cracking; shaping; size-effect; statistical nature of strength; ultrasonic cutting; Weibull distribution.

In mechanical shaping processes for brittle solids, materials are removed by the propagation and intersection of cracks. To control the resulting surface finish, the extent of cracking is localized by loading the surface in very small regions, usually with small abrasive grains. Thus, in analyzing such processes as erosion and ultrasonic cutting, we have to examine the fracture patterns produced by small hard indenters.

As a starting point, it is shown that fracture loads for indenters subjected to normal force may be predicted from conventional strength tests by using Weibull's statistical treatment of brittle strength. It is then shown that Weibull's procedures may be extended to predict the distribution of fracture location in brittle solids. For the case of a spherical indenter under normal and tangential forces, many cracks may form as the load is increased. It is shown that the location of the outermost of these cracks may be predicted. Estimates may also be made of the depth of cracking and thus the extent of the cracking produced by a single contracting particle may be described.

These results may be applied directly to study the process of erosive shaping. The influence on volume removal of changes in the velocity and size of the impacting particles is predicted and shown to be in accord with experiment. Many other features of the erosion process may be described including a transition to "ductile" behavior in the case of glass when the impacting particles are small enough. The analysis of ultrasonic cutting presents greater difficulty because the distribution in size of the abrasive grains is of great importance. However, predictions may be made for the influence of load, grain size, and material properties on the rate of volume removal and these are shown to be in general accord with experiment.

**Sonic machining of ceramics,** W. B. Campbell, *SP348*, pp. 133-139 (May 1972).

**Key words:** Abrasive; ceramic machining; sonic machining; vibrational machining; wheel machining.

The effect of 10 kHz sonic vibrations on the shaping and finishing of fired ceramic shapes was investigated to identify optimum machining conditions commensurate with product and surface quality. Sonic motors, developed at The Ohio State University and with outputs up to 15 horsepower, were used to activate the machine tool. Significant improvements in tool wear were observed in impact-tuned systems that produced removal rates greater than 45 cu in per min. Template and profile tooling were successfully used to obtain open cutting surfaces. Over 3,000 test cuts provided the data necessary to identify optimal parameters of operation.

**Environment-sensitive machining behavior of nonmetals,** A. R. C. Westwood and R. M. Latanision, *SP348*, pp. 141-153 (May 1972).

**Key words:** Adsorption; ceramics; drilling; environmental effects; fracture; glasses; machining; mechanical behavior.

Liquid environments can influence the efficiency of machining nonmetallic solids in a variety of ways, e.g., by serving as lubricants, coolants, or particle dispersants. More importantly, however, certain environments can markedly increase or decrease the hardness of the near-surface regions of such solids, and thereby exert a profound influence both on the rate of material removal and on tool life. Because of its technological potential, the characteristics and possible mechanisms of this latter phenomenon—the Rebinder effect—receive primary consideration in this paper.

For crystalline ceramics, Rebinder effects in machining arise because of the influence of the environment on near-surface dislocation behavior. Effects resulting from adsorption-induced changes in the surface free energy of the solid are of minor importance. Rebinder effects can also occur in noncrystalline solids, however, and recent observations on such effects in various glasses are described. The possibility that these effects are caused by a stress-plus-chemisorption-induced redistribution of sodium ions in the near-surface region is discussed.

The importance of considering the total cutting system, environment-solid-tool, in any account of environment-sensitive machining is stressed, for environments which facilitate material removal when one type of tool is used can be detrimental to the effectiveness of another tool with a different cutting action.

**Shaping or figuring ceramic surfaces by ion-beam bombardment,** P. W. Levy, *SP348*, pp. 155-168 (May 1972).

**Key words:** Figuring; ion-beams; optical surfaces; polishing; radiation damage; sputtering.

The shaping or figuring of glass and ceramic surfaces by ion-beam erosion is a relatively new technique. All operations are carried out in a vacuum. Usually the optic is bombarded by a collimated beam of rare gas ions whose energy is between 1-100 keV. Selected areas can be eroded by electrostatically deflecting the beam or, less conveniently, by moving the optic. The erosion area can be controlled by focusing the beam with electrostatic or magnetic lenses. The basis of the erosion process is the physical phenomenon known as sputtering. This occurs when the incident ions scatter elastically with atoms near the surface of the target and some of the displaced atoms, after participating in one or more collisions, acquire sufficient velocity to escape from the solid. Other dislodged atoms become interstitials and, together with vacancies created in the recoil process, create a radiation-damaged layer just below the eroding surface, whose thickness is roughly the range of the bombarding ions. For ceramic materials, typical erosion rates are on the order of angstroms/ $\mu\text{amp}/\text{cm}^2/\text{min}$  and increase with increasing angle of incidence. Ion-beam currents up to 100  $\mu\text{amp}/\text{cm}^2$  are practical. Under these conditions, the material struck by the beam may reach temperatures between 300 and 700 °C. The maximum lattice disruption occurs at a depth of one incident ion range from the original surface just as the eroding surface reaches this point. Additional bombardment does not increase the damage beyond this maximum. Furthermore, the damage is minimized by using bombardment conditions which maximize the temperature in the target. It is not known if there are any radiation damage effects which reduce the usefulness of ion-beam figured optics. At the moment, it would appear that ion-beam figuring is a practical technique for "touching up" conventional optics and, more importantly, for fabricating nonspherical or



nonaxially symmetrical optics. Also, the ion-beam erosion process is particularly amenable to computer control.

**The effect of sputtering on surface topography and strength of ceramics**, R. W. Rice, *SP348*, pp. 171-187 (May 1972).

Key words: Carbides; glass, ion beam sputtering; nitrides; oxides; RF sputtering; strength; surface finish; twins.

The topography developed as a result of RF sputtering on a variety of ceramic surfaces is described showing that surface cracks, scratches, pits, etc., are fairly rapidly rounded out. Generally, this occurs without differential grain boundary sputtering. However, some bodies develop a rough finish due to nonuniform microstructural removal. Limited trials with ion beam sputtering show it also rounds cracks, etc., but does not develop a rough finish on bodies that will with RF sputtering.

Because of the rounding of stress concentrating features and generally similar effects on single and polycrystalline bodies, sputtering was investigated as a substitute for flame polishing, but with much wider applicability. Flame polished strengths were not obtained. However, some materials (e.g.,  $\text{MgAl}_2\text{O}_4$ ) do show greater improvements in strengths than others (e.g.,  $\text{Al}_2\text{O}_3$ ) as a result of sputtering. These differences will be discussed and results compared with other methods of surface finish.

Both the detailed nature of the sputtered surface as well as enhancement of grain boundaries and other microstructural features under certain conditions indicate that sputtering may also be useful as an etching technique.

**Computer controlled ionic polishing of optical surfaces**, J. W. Douglass, *SP348*, pp. 189-192 (May 1972).

Key words: Computer controlled process; ion beam technology; ionic polishing; optical fabrication; optical scatter; sputtering.

Results of the development of an ionic polishing investigation are described. During this investigation many controlled polishing experiments were performed. The results of two of these experiments are presented. In the first of these, a 0.203 m diameter optical flat of fused silica was polished to a diffraction limited surface quality of 95A (9.5 nm) rms. The second experiment described was the conversion of a 0.203 m diameter Cervit sphere into an  $f/5$  paraboloid of diffraction limited quality by using analytical expressions to generate the removal distribution. The ionic polishing process was computer controlled for this experiment. The temporal stability and optical scatter performance of ionically polished surfaces has been determined to be as good as or better than conventional surfaces.

**Arc, laser, and electron beam machining of ceramics**, R. W. Rice, *SP348*, pp. 193-195 (May 1972).

Key words: Arc machining; cutting; drilling; electron beam machining; laser machining; shaping; thermal shock control.

The various types of arc, laser, and electron beam machining, the considerations that are required in their operations, and some of the applications for which they have been tried or used, are briefly reviewed. The most general consideration is whether thermal shock and stress cracking will be a problem. The environmental and material parameters, which vary substantially with the types of these different machining processes, can also be quite important. Meeting the requirements of all these considerations does limit the versatility and applicability of these techniques. Nevertheless, they deserve consideration for a variety of applications.

**The techniques and mechanisms of chemical, electrochemical, and electrical discharge machining of ceramic materials**, D. W. Lee and G. Feick, *SP348*, pp. 197-210 (May 1972).

Key words: Ceramic materials; chemical machining (CHM); electrical discharge machining (EDM); electrochemical machining (ECM); intermetallic compounds.

Electrochemical Machining (ECM), Electrical Discharge Machining (EDM), and Chemical Machining (CHM) techniques have not been extensively used as a material removal process for ceramics. The fact that these processes are not dependent upon the hardness of the workpiece should make them attractive for the shaping of ceramics. However, ECM and EDM techniques are limited to material with reasonably good electrical conductivity while CHM may be limited by the availability of effective etchants and the nature of the ceramic itself.

The theory and techniques of chemical, electrochemical, and electrical discharge processes will be reviewed. The variables and important parameters of the material removal processes will be discussed, including etchants and mask techniques for chemical milling; current-voltage characteristics, dielectric fluids, electrode materials, etc., for EDM; electrolytes, gap effects, current density, etc., for ECM. The available information and experiences developed on metals and alloys will be used to examine the applications and limitations of these processes to ceramic materials. Where possible, the effects of the material removal process on the surface condition, microstructure, and subsequent material properties will be pointed out. Finally, comments will be made on the technical and economic feasibility of ECM, EDM, and CHM processes for the shaping, cutting, and finishing of crystalline ceramics.

**Improvements in the surface finish of ceramics by flame polishing and annealing techniques**, M. J. Noone and A. H. Heuer, *SP348*, pp. 213-232 (May 1972).

Key words:  $\alpha\text{-Al}_2\text{O}_3$ ; annealing; flame-polishing; reinforcements; ruby; sapphire; strength; surface perfection.

Improvements in the surface perfection (i.e., "smoothness") of ceramics can be achieved by thermal treatments at temperatures where material transport may be induced at the surface. Such treatments include annealing in controlled environments, where surface diffusion, vapor transport mechanisms, etc., may be active, and flame polishing, where a thin layer at the surface of the material is melted, allowed to flow freely, and then resolidified.

The effects of these treatments on the surface of single crystals of  $\alpha\text{-Al}_2\text{O}_3$  are reviewed in this paper. The most sensitive assessment of the degree to which surface perfection is attained is the measurement of the strength of the treated crystals; for this reason, strength data are used extensively to characterize the thermal treatments described. In the case of flame polishing, it found that a sufficient degree of surface perfection can be attained so that the strength is no longer limited by surface defects (the usual experience with ceramics) but by defects within the material. The technological significance of high strength  $\text{Al}_2\text{O}_3$  filaments for reinforcement of metals and the unfortunate deterioration of the surface in these applications is briefly described.

**Healing of surface cracks in ceramics**, F. F. Lange, *SP348*, pp. 233-236 (May 1972).

Key words: Abrasive machining; ceramics; crack healing; sintering; surface damage.

Grinding, cutting, thermal shocking, impacting, and rough handling all introduce surface cracks that degrade the strength of ceramics. Within the last year, it has been shown that, once introduced, these cracks can be eliminated by either resintering the damaged ceramic component for the case of oxides or oxidizing the component for the case of materials such as SiC.

Results of crack healing experiments, performed on  $\text{Al}_2\text{O}_3$ , ZnO, and SiC will be reviewed. The technical implications of these results will be discussed as related to abrasive machining.

**Flame polishing of flat oxide bars**, P. F. Becher and R. W. Rice, *SP348*, pp. 237-244 (May 1972).

**Key words:** Flame polishing; glass; rutile; sapphire; spinel; strength; surface characterization; twinning.

Some of the problems and limitations of flame polishing flat bars are discussed. Results are presented for single crystal,  $\alpha\text{-Al}_2\text{O}_3$ , as well as for more limited trials of  $\text{MgAl}_2\text{O}_4$ ,  $\text{TiO}_2$ , and soda lime glass. The wide variability of strength is partially related to variations in surface, but twinning also appears to be important in sapphire and  $\text{TiO}_2$ . Preliminary results on twin sources and their effect on strength of sapphire are discussed.

**Continuous flame polishing of sapphire filament**, J. T. A. Pollock, *SP348*, pp. 247-256 (May 1972).

**Key words:** Characterization; continuous flame polishing; sapphire filament; strength enhancements.

Continuous flame polishing of nominal  $2.5 \times 10^{-4}$  m diameter single crystal sapphire filament oriented with the c-direction parallel to the filament axis has resulted in considerable enhancement of the tensile fracture strength. Optimum increases of approximately  $1.1 \times 10^9$  N/m<sup>2</sup> ( $1.6 \times 10^5$  psi) have been obtained on flame polishing many lengths of filament exhibiting as-grown tensile strength of  $2.2 - 2.8 \times 10^9$  N/m<sup>2</sup> ( $3.2 - 4.0 \times 10^5$  psi). Flame polishing was carried out in a continuous manner at  $6.3 \times 10^{-4}$  m/sec using an oxygen/hydrogen flame. Data are presented which suggest that the enhancement is not entirely dependent on the production of a more perfect  $\text{Al}_2\text{O}_3$  surface. Increases in strength of approximately  $5.5 \times 10^8$  N/m<sup>2</sup> ( $8 \times 10^4$  psi) are reported for filament which has passed through flames not sufficiently hot for surface melting to occur. Maximum strength enhancement is obtained when the oxygen/hydrogen flame temperature is such that an axial molten zone two to three times the filament diameter is produced at the filament surface. When the flame temperature is too high, the geometric integrity of the filament is lost and an apparent fall in tensile strength from the peak value is observed.

Metallographic evidence is presented indicating that the molten zone has a radial depth of less than  $6.5 \times 10^{-6}$  m. Scanning electron microscopy and related surface analysis studies are reported which confirm that optimum polishing results in a smoother filament surface. Experiments to determine the state of stress in the filament before and after polishing are described.

The relative contributions to the reported tensile strength enhancement of thermal strain relieving, thermally activated atomic diffusion leading to blunting of possible fracture sources, and the creation of a more perfect  $\text{Al}_2\text{O}_3$  surface are discussed.

**Preparation of smooth crystalline, damage free, sapphire surfaces by gaseous etching**, W. A. Schmidt and J. E. Davey, *SP348*, pp. 259-265 (May 1972).

**Key words:** Crystalline sapphire surfaces; fluorinated-

hydrocarbon etch; fluorotrichloromethane; freon etching; hydrogen annealing; sapphire; sapphire substrates; sapphire surface preparation.

Sapphire has a combination of properties such as relative chemical inertness, exceedingly high resistivity, optical transparency, and crystalline structure that suggests its use as a substrate material for various semiconductor devices. Its successful use for silicon vapor phase epitaxy substrates indicates that similar results might be possible with other semiconductors. Previous epitaxial studies have shown that surface crystalline disorder and topographic imperfections inhibit epitaxial growth; therefore, highly polished, well ordered sapphire surfaces were needed. Mechanical polishing alone is insufficient as it results in cold flow and work damage.

Initial experiments in removing surface damage were performed with hot phosphoric acid and with hydroxide etches. Undesirable preferential etching was observed for both processes and the processes did not seem amenable to the routine production of high quality surfaces. Two other surface treatments for which successful results have recently been reported were investigated.

The first was a hydrogen firing technique in which the substrates were heated in hydrogen in an Mo wound resistance furnace at 1500 °C. The second was a simple laboratory process in which the sample is heated by means of RF heating of a carbon susceptor to 1350 °C in an atmosphere of helium and fluorotrichloromethane (Freon-11). Commercial reagents were used throughout and a fused quartz tube was used for the reaction chamber for the second technique.

Reflection electron diffraction (RED) was used to determine the surface crystalline order, and electron microscopy (EM), using high resolution replication techniques, was used to examine the topography structure of the surfaces. A number of different substrates from various industrial sources, with different surface topographies and different orientations, were used.

Hydrogen firing at 1500 °C results in an etch rate of  $0.1 - 10^{-6}$  m/min. Firing for times up to 45 min did not produce consistent surfaces on the 0, 60 or 90° orientations. While hydrogen firing did produce high quality, well ordered crystallograph surfaces by RED, their topographic condition was poor. Resolvable surface structures could be detected on some with standard optical microscopy (200x, dark field) and for all high resolution EM measurements. The final surface finish quality was related to the quality of the prefired surface, indicating that complete damage removal was not accomplished.

Freon firing at 1350 °C resulted in an etch rate of  $1.5 - 10^{-5}$  m/min. This technique consistently produced well ordered, high quality surfaces for the 60 and 90° oriented surfaces. EM viewed 60 and 90° freon-fired surfaces had no resolvable surface structure after a 5 min etch and were well ordered crystallographically as measured by RED. The same etch produced strongly etched surfaces on 0° oriented material.

**The strength of gas polished sapphire and rutile**, R. W. Rice, P. F. Becher, and W. A. Schmidt, *SP348*, pp. 267-269 (May 1972).

**Key words:** Chemical polishing; rutile; sapphire; spinel; strength; twinning.

Surface polishing of  $\alpha\text{-Al}_2\text{O}_3$  using a helium-freon gas mixture at elevated temperatures is shown to yield bend strengths comparable to flame polished sapphire. However, the gas polishing process proved to be more versatile as



evidenced by the success with flat bar surfaces. Further, the process can be readily applied to some other materials as demonstrated by the substantial improvements in the strength of  $\text{TiO}_2$  after gas polishing. Limited attempts at polishing other ceramic materials are also discussed, as well as observations on strength variations and fracture behavior.

**Analysis and characterization of ceramic surfaces for electronic applications**, R. C. Sundahl and L. Berrin, *SP348*, pp. 271-290 (May 1972).

**Key words:** Aluminum oxide; Auger electron spectroscopy; crystallographic texture; ion microprobe; scanning electron microscopy; substrates; surface defects; surface segregation; thin film adhesion; thin film circuit imperfections.

The criteria which are used to evaluate the surfaces of ceramic substrates for use in the electronics industry must be related to the specific application of the surface. This article emphasizes one such application—the use of a ceramic surface as a support for complex thin film conductor patterns which serve to interconnect silicon integrated circuit chips. Those ceramic surface parameters which are found to be critical to this application are (1) topographical properties, (2) chemical properties, and (3) crystallographic properties.

These properties are characterized using such tools and techniques as optical, transmission electron and scanning electron microscopy, profilometry, electron microprobe analysis, ion microscope analysis, Auger electron spectroscopy, and electron diffraction. Special emphasis is placed on the relationship between the results of such analyses and the performance of the surface as part of the SIC interconnect system.

**Surface characteristics of ceramic substrates for hybrid and microwave electronic circuits**, J. K. Emery, *SP348*, pp. 293-300 (May 1972).

**Key words:** Camber; ceramic; fired; flatness; ground; lapped; microwave; polished; roughness; substrate; surface; thick film; thin film; waviness.

Several methods currently used for finishing ceramic substrates in ready-for-deposition state are discussed, including firing, glazing, burnishing, grinding, lapping, and polishing. Each method tends to exhibit a different and typical combination of surface characteristics, such as variations in thickness, parallelism, camber, waviness, roughness, and localized defects; each of these in turn may influence the deposition process, performance, and reliability. Analysis of some typical surface details, particularly roughness and waviness, as significant surface factors capable of affecting process or function, is presented with comments on instrumentation and measurement procedures.

Significant differences exist in the use of terms relating to substrate surfaces and their characteristics; a need is indicated for more particularized use of such terms and for recognition of uniform definitions. Clarification of terminology may facilitate improved communications and measurements, which in turn may correlate with current and future requirements in circuit production. Several existing applicable standards are referenced, and definitions of terms are suggested. A number of choices of surface characteristics are presented which may be related with process controls and function, but no recommendations for particular values of surface details are intended.

**Ceramic surface texture by reflective replica technique**, W. C. Lo, *SP348*, pp. 301-307 (May 1972).

**Key words:** Alumina substrates; surface replica; surface texture.

Surface texture is a parameter of general concern in the study of thin film metallizing adherence on ceramic substrates. It refers to the geometrical character of the surface irregularities recurring many times across the ceramic surface tending to form a pattern. In this context, surface texture is determined by the size, shape, arrangement, and distribution of the surface constituents.

This note presents a convenient method by which the surface texture of ceramic substrates can be visually assessed and recorded photographically using a simple metallographic microscope.

Examples in applying this technique for distinguishing and differentiating surface textures of different types of ceramic substrates are given. Use of the technique for identifying surface defects is also shown.

The simplicity of the method should warrant its use for monitoring the physical surface quality of ceramic substrates.

**Quantitative surface finish characterization by CESEMI**, E. W. White, H. A. McKinstry, and A. Diness, *SP348*, pp. 309-316 (May 1972).

**Key words:** Ceramic materials; CESEMI (Computer evaluation of scanning electron microscope images); digital magnetic tape recordings; profilometer; profilometer rasters; quantitative characterization; scanning electron microscope; surface finish analysis; surface morphology; surface roughness; surface topography; three-dimensional images.

A feasibility for quantitative characterization of surface finishes based on the computer evaluation of scanning electron microscope images (CESEMI) has been established. Measurement of the number, size, shape, and orientation of iso-intensity (or selected intensity interval) regions constitute the basic analysis. Brightness in SEM images varies as a function of the steepness of slope of the surface at a given point. In their analysis, the characteristics of grooves, pits, ridges, etc., can be studied separately. Detailed interpretation of the results is not attempted in this preliminary study.

A feasibility for recording and analyzing profilometer rasters has also been demonstrated. Such recordings are, in essence, true three-dimensional images of surface topography insofar as the profilometer stylus faithfully follows the surface morphology. Analysis of these profilometer recordings by the basic CESEMI computer programs yields direct descriptions of the topography. The SEM image and profilometer "image" analyses appear to be complementary techniques. One obvious advantage of the SEM image analysis is that it is a no-contact technique; hence, there are no problems introduced by stylus damage.

**An assessment of surface and subsurface damage introduced in ceramics by semifinish grinding operations**, B. G. Koepke, *SP348*, pp. 317-332 (May 1972).

**Key words:** Ceramics; etch pits; fracture; grinding damage; plastic deformation; surface condition; surface grinding.

The nature and extent of grinding damage introduced by surface grinding a number of ceramics having widely varying mechanical properties have been studied. Surface damage has been characterized by optical and electron microscopy, and subsurface damage has been observed using etch pit techniques. Grinding damage was found to depend strongly on wheel type and rate of material removal as well as on the mechanical behavior and microstructure of the workpiece. The results indicate that grinding damage is

mainly composed of mixtures of three types depending on the mechanism of material removal.

When material is removed efficiently from low impact resistance ceramics (e.g., magnesium oxide and ferrite), the surfaces are generated by brittle fracture and are composed of regions of transgranular and intergranular fracture. When grinding is inefficient, i.e., when the grinding wheel loads up, material is removed by plastic flow. The resultant surfaces on deformable ceramics (e.g., magnesium oxide, ferrite, and silicon) are smooth and burnished but may contain thermal cracks due to the heat generated. In this instance, subsurface damage consists of a discrete, highly deformed layer containing cracks in most cases.

When material is removed efficiently from high impact resistance, nondeformable ceramics (e.g., alumina and boron carbide) material is removed by plastic flow and by transgranular and intergranular fracture. The presence of extensive plastically flowed regions on the ground surfaces of extremely hard ceramics is surprising and points out the extremes of stress and temperature existing under the wheel-workpiece interface during a grinding pass.

**Observations on mechanically abraded aluminum oxide crystals by transmission electron microscopy**, B. J. Hockey, *SP348*, pp. 333-339 (May 1972).

**Key words:** Abrasion; aluminum oxide; dislocations; ion-bombardment; microtwins; scanning electron microscopy; subsurface damage; transmission electron microscopy.

Use of the argon ion-bombardment thinning technique has made possible the examination of the near surface regions of mechanically abraded aluminum oxide by transmission electron microscopy. Observations on diamond-polished (0.25  $\mu\text{m}$ ), alumina-polished (0.3  $\mu\text{m}$ ), and diamond-ground specimens have shown that subsurface damage as well as surface damage is typically produced.

Specifically, mechanical polishing introduces relatively high densities of dislocations to a depth of approximately 1  $\mu\text{m}$  from the original surface. The dislocations are generally in the form of half-loops and are clearly associated with surface scratches produced by individual abrasive particles.

The magnitude of residual surface stresses and the irregular surface topography produced by grinding necessitated the removal of at least 2–4  $\mu\text{m}$  from the original surfaces. At this depth, both the nature and extent of subsurface damage in polycrystals varied from grain to grain. Most grains contained either tangled dislocation arrays or microtwins (either basal or rhombohedral). A number of grains, however, were found to be completely free of damage and may correspond to regions below fracture surfaces which are apparent in observations of ground surfaces by scanning electron microscopy.

**Acoustic emission monitoring of surface-damaged ceramic materials**, L. R. Bunnell, J. C. Crowe, and P. E. Hart, *SP348*, pp. 341-342 (May 1972).

**Key words:** Acoustic emission; glass; Lucalox; Pyroceram; surface damage.

The acoustic emission response of Lucalox, fused silica, single crystal alumina, Pyroceram, and soda-lime-silica glass to surface damage is reported. Low temperature annealing at 200 °C reduces the response levels; annealing at 400 °C removes all of the induced acoustic activity.

**Effects of surface finishing on mechanical and other physical properties of ceramics**, R. J. Stokes, *SP348*, pp. 343-352 (May 1972).

**Key words:** Ceramics; cracks; dislocations; electrical pro-

perties; electro-optical; ferrite; machining; magnetic properties; mechanical properties; optical properties; residual stress.

This paper reviews the effects of mechanical finishing operations on the physical properties of ceramics. Ceramic machining results in a defective surface containing cracks, dislocations, point defects, and residual stresses. The relative significance of these defects depends on the physical property of interest. The mechanical properties of single crystals are sensitive to dislocations (semibrittle) and surface cracks (brittle); the mechanical properties of polycrystals are sensitive to surface cracks; the electrical properties of semiconductors are sensitive to surface trapping sites; magnetic, piezoelectric, and optical properties are particularly sensitive to residual stresses. To optimize physical properties, these defects must be eliminated by mechanical lapping, chemical etching, or thermal annealing.

**Strength effects resulting from simple surface treatments**, H. P. Kirchner, R. M. Gruver, and R. E. Walker, *SP348*, pp. 353-363 (May 1972).

**Key words:** Abrasive machining; alumina ceramic; chemical polishing; crack healing; delayed fracture; glazing; humidity; refiring; strength; surface flaws; surface treatments; thermal shock.

In well made polycrystalline alumina ceramics subjected to external loads, fracture originates, in almost every case, at surface flaws rather than at volume flaws. This susceptibility to surface flaw failure has been reliably established in experiments in which compressive surface layers were used to obtain substantial improvements in strength. Knowing that the failures occur at surface flaws, the artificial introduction of surface flaws can be used to obtain an understanding of the ways in which surface flaws affect the strength. Additional information can be gained by using simple treatments to change these artificial surface flaws and by observing the effect of these treatments on the strength.

In the present investigation, artificial flaws were introduced by single point tools, abrading, thermal shock, and abrasive machining. The flaws were treated by refiring, chemical and flame polishing, chemical etching, glazing, and prolonged storage in various environments.

The changes in the flaws were characterized by microscopy and to a limited extent by profilometry. Both flexural and tensile strengths were measured. The effects of the treatments are discussed in terms of changes in the average strength and variations in the distributions of the individual strengths.

**The effect of grinding direction on the strength of ceramics**, R. W. Rice, *SP348*, pp. 365-375 (May 1972).

**Key words:** Carbides ceramics; fracture; grain size; grinding; hardness; mechanical testing; nitrides; oxides; strengths.

It is shown that grinding bars in a direction parallel with the tensile axis has limited effects on their strength while grinding perpendicular to the tensile axis may have no effect or can reduce strengths as much as 50 percent. In single crystals, the reduction in strength generally increases with the hardness of the material but can also depend on crystallographic orientation. In polycrystalline bodies, the reduction also depends a great deal on grain size, with the effect generally increasing with decreasing grain size. Also the effect tends to be greater in polycrystalline bodies that are weaker than normal. The effect of grinding direction on



strength is attributed to stress concentrations due to grinding stria, whose continuity and depth generally increase with hardness. The severity of these stria tends to increase as the amount of plastic deformation in the machined surface decreases. The amount of plastic deformation is shown to vary approximately inversely with hardness. The effect of varying strength with grinding direction on the interpretation of various tests is discussed.

**The influences of material removal on the strength and surface of an alumina**, H. S. Starrett, *SP348*, pp. 377-388 (May 1972).

Key words: Alumina; surface finish; surface treatments; Weibull.

Southern Research is conducting a quantitative investigation of test methods used to evaluate brittle materials. The material for this study is a high purity, high density alumina manufactured by Coors Porcelain Co. of Golden, Colo. The primary scope of the total program is a study of test methods, scaling laws, and surface finish effects. The scope has been broadened to include the effects of property interactions on strength and the relationships between micro and macro characterization and the mechanical properties.

Initial tensile and flexural data indicated that surface finish had no effect on the tensile strength of this particular alumina. Since this was contrary to generally accepted results, considerable effort has been expended in investigating this phenomenon. It has been postulated that the lack of an effect may have been due to subsurface damage that occurred during the grinding operations.

The investigations into surface/subsurface damage have focused into four principal areas. Microstructural characterization has been used to characterize the surfaces of interest, to look for evidence of damage, and to look for microstructural events which may be normalizing the data. A study of fracture source distribution has been made in order to determine the depth of damage which would have a significant effect on the flexural data. Surfaces have been and are being subjected to different treatments such as refiring in modified environments and deep lapping in order to define the nature of the surface/subsurface damage, if it exists.

The microstructural work has not revealed any obvious damage; however, it was found that even by proceeding from a shop grind to a metallurgically lapped surface, certain features such as exposed pores, interfaces between alumina matrix and second phase, and evidence of the original ground surface did not totally disappear. The study of the fracture source distribution provided quantitative evidence that damage on the order of 0.005 in (approximately five maximum grain diameters) would have a significant effect on the flexural data. Results from the surface treatments, deep lapping, and refiring show that these different preparations did not affect the flexural strength of the material. Other indirect evidence (statistical data) show this material to be insensitive to surface effects within the range of surface finishes investigated.

**The effect of grinding variables on the strength and surface finish of alumina**, R. Sedlacek, F. A. Halden, and P. J. Jorgensen, *SP348*, pp. 391-397 (May 1972).

Key words: Alumina; diamond grinding; surface finish; tensile strength.

The tensile strength of alumina is used as a criterion for the evaluation of the effects of variables encountered in diamond grinding of ceramics. The variables studied include the grit size of diamond, rate of material removal, and spark-

out. The difference in performance of natural and synthetic diamond is shown, and the feasibility of dry grinding is discussed. The ground surfaces were examined using profilometry, and transmission electron and scanning electron microscopy. The strengths of test specimens having ground or as-fired surfaces are compared.

**Edge effect on the modulus of rupture of ceramic substrates**, W. C. Lo, *SP348*, pp. 399-400 (May 1972).

Key words: Alumina substrate; edge damage; flexural strength.

Because of its simplicity, the modulus of rupture (or flexural strength) test is often used to evaluate the mechanical strength of ceramics. For large flat substrates, the natural tendency is to test specimens cut from the substrate.

Depending on the method of cutting and the resulting edge condition of the specimen, the flexural strength can be significantly different. This is illustrated by 3-point loading data on CO<sub>2</sub>-laser-scribed and diamond-sawed specimens. The modulus of rupture of a laser-cut sample is about 70 percent of that of a diamond-sawed sample.

**SP349. Heavy-atom kinetic isotope effects, an indexed bibliography**, M. J. Stern and M. Wolfsberg, *Nat. Bur. Stand. (U.S.)*, Spec. Publ. 349, 39 pages (June 1972).

Key words: Author index; bibliography; heavy-atom isotope effects; isotope effects; kinetic isotope effects; reaction kinetics; subject index.

A bibliography of heavy-atom kinetic isotope effects has been compiled covering the complete literature from the earliest entry found (1911) through 1965. Review articles and theoretical papers are listed through 1968. The bibliography is divided into a list of the references, an author index and a subject index. The subject index has been annotated to describe, in brief, the type of reaction being observed. The following areas have been excluded: geochemistry (except for specific laboratory reactions), living systems, mass spectrometry and electron impact, electrochemistry, diffusion-controlled processes, hot-atom chemistry, photochemistry involving selective excitation of isotopes and processes involving no chemical change.

**SP351. Analytical chemistry: key to progress on national problems**. Proceedings of the 24th Annual Summer Symposium on Analytical Chemistry sponsored by *Analytical Chemistry*, ACS Division of Analytical Chemistry, and NBS Analytical Chemistry Division, and held at the National Bureau of Standards, Gaithersburg, Md., June 16-18, 1971, W. W. Meinke and J. K. Taylor, Editors, *Nat. Bur. Stand. (U.S.)*, Spec. Publ. 351, 481 pages (Aug. 1972).

Key words: Agriculture; air pollution; analytical chemistry; biomedicine; clinical chemistry; electronics; oceanography; solid state; water pollution.

This book is the formal report of the proceedings of the 1971 Summer Symposium in Analytical Chemistry held at the National Bureau of Standards, June 16-18, 1971, and cosponsored by the Analytical Chemistry Division of NBS, *Analytical Chemistry*, and the American Chemical Society's Division of Analytical Chemistry. It contains six invited papers by subject matter experts comprehensively reviewing urgent research problems for which advanced analytical techniques need to be developed in the important areas of agriculture, air pollution, clinical chemistry and biomedicine, oceanography, solid state research and electronics, and water pollution. Summaries of related discussions by leading analytical chemists serving as panel members or in attendance at the Symposium are included. Hundreds of important analytical problems retarding progress in

these important areas are described and extensive references are given to permit a deeper insight into the problem areas. Accordingly this volume should not only stimulate interest in important problems but should provide a valuable guide for highly relevant analytical research for some time to come. *These proceedings include the following papers (indented):*

**The chemical analysis of things as they are,** G. E. F. Lundell, *SP351*, pp. 1-18 (Aug. 1972).

**Opportunities for analytical chemistry in solid state research and electronics,** R. A. Laudise, *SP351*, pp. 19-77 (Aug. 1972).

**Key words:** Analytical chemistry; electronic materials; materials characterization; solid state research; stoichiometry; trace analysis.

Current practices and problems in analysis in solid state research and development are reviewed. A plea that the analyst assume a broadened responsibility for characterization of materials is made. Examples of solid state problems which were caused by inadequate appreciation and application of analysis are given. In particular, it is pointed out that trace analysis at and below the ppb level, the careful assessment and mapping of physical perfection by x-ray and related techniques and the use of solid-state physical measurements such as conductivity and magnetic resonance will become more important in the future. Mapping techniques and perfection techniques are reviewed in some detail. Recent new methods of stoichiometry assessment are described, and it is suggested that the determination of perfection and defects should become an orderly subdiscipline under the aegis of analytical scientists. The case is made that, insofar as both research and technological progress in solid state and electronics are rate limited by the availability of materials with appropriate properties, it is limited in many cases by our ability to characterize materials. It is concluded that with a modest reorientation of viewpoint and disciplinary content, analytical science could become the core discipline of materials characterization.

**Analytical problems in biomedical research and clinical chemistry,** G. N. Bowers, Jr., and J. Meyer II, *SP351*, pp. 77-159 (Aug. 1972).

**Key words:** Biomedical research; clinical chemistry; clinical enzymology; enzyme standardization; health science; hospital laboratory; medical research.

The key to progress in national problem areas in health rests over the long term with the success of our country's biomedical research efforts. Analytical chemistry can contribute significantly to these vital efforts by providing the sound base of quantitative chemical measurements required by these health investigations. But health research must not be construed too narrowly. The responsibility for the chemistry related to our national health needs cannot be assigned exclusively to any one scientific group. Indeed, some of the most profound insights may well originate far beyond the usual confines of the medical research community. This will be especially true in the environmental health areas where analytical chemists from many fields will make important contributions.

The elucidation and cure of disease processes are becoming ever more dependent upon chemistry. As a direct result of successful recent past biomedical research, the demand for diagnostic chemistry tests has increased faster than almost any other health service. Service chemistry is thus closely related to medical research and also medical education activities, as will be demonstrated by experience with transaminase assays in heart attacks and calcium determinations in hyperparathyroidism.

To support the rational development and utilization of automated analytical systems in health service and research laboratories, there is a clearly defined need for high purity standard reference materials and certified reagents. Clinical laboratories urgently require the development of high accuracy referee methods to improve the specificity and systematic bias of routine methods.

In short, *life is a chemical system*. Meaningful quantitative chemical measurements are essential to our understanding of its complex internal interactions as well as our profound interdependency upon other life forms in the environment.

**Analytical problems in agricultural science,** G. W. Irving, Jr., and W. C. Schaefer, *SP351*, pp. 161-243 (Aug. 1972).

**Key words:** Agricultural pollution; agricultural products analysis; agricultural science; amino acid analysis; biomedical research; clinical chemistry; diagnostic chemistry; food analysis; pesticide residue analysis.

This paper presents a review and analysis of the widespread applications of analytical chemistry and analytical instrumentation in the research and regulatory programs of the Agricultural Research Service of the Department of Agriculture. Analytical chemistry is one of the essential sciences needed in advancing the commodity and people-oriented programs which can achieve the national goals of the Department. Chemical analysis will be shown to play a vital role in assuring an adequate supply of farm and forest products and in assuring the consumer a better product while minimizing costs for processing and distribution. In people-oriented programs, such as consumer health, safety and pollution abatement, analytical methodology is the key procedure for providing the basic data to get action programs into motion.

Along with the far-ranging applications of analytical chemistry in agriculture come many unsolved analytical problems. In fact, few agricultural scientists will admit complete satisfaction with any of their current methodologies. Yet some problems are more important than others. An assessment of these problems is made including an analysis of their relative importance in conjunction with the urgent needs of agriculture. Possible ways of classifying or categorizing these problems will be suggested. For example, amino acid analysis touches almost every branch of agricultural science whereas pesticide analysis is more restricted but has a great many more complexities. For any given pesticide, methodologies may be needed for controlling its application and for measuring its residues in free and bound form, its metabolites, trace contaminants, and the inert ingredients in its formulation.

Other problems are discussed for which there appears no current solution. This will challenge the ingenuity and creativity of analytical chemists in the future.

**Analytical problems in air pollution control,** A. P. Altshuler, *SP351*, pp. 245-295 (Aug. 1972).

**Key words:** Air pollution; air quality instrumentation; air quality measurements; anion analysis; Clean Air Act; elemental analysis; measurement of atmospheric gases and vapors; measurement of atmospheric particles.

The role of measuring techniques in activities ranging from research to regulatory activities of the Environmental Protection Agency will be discussed. Field and laboratory instruments and manual techniques will receive consideration. Both point-sampling and remote types of instrumentation developments will be reviewed. Chemical and physical transformations contribute to the formation of new or



modified pollutant species. Air quality measurements must be capable of properly following such transformations. Especial emphasis needs to be given to the conversion of gaseous into various submicron particulate species. The mass, particle-size distribution and details of chemical composition of these particles is required. Examples will be given of new and improved types of air quality measurements, stationary source and mobile source emission measurements which may be needed to meet air quality and emission standards.

**Analytical problems in water pollution control**, K. H. Mancy, *SP351*, pp. 297-430 (Aug. 1972).

**Key words:** Aquatic environment; environmental analysis; trace analysis; water analysis; water pollution; water pollution control.

The analytical chemistry of natural and waste waters requires subtle correlation between theory and experience, an insight into the nature and mode of action of interferences, and the ability to interpret analytical results in correlation with pertinent field observations. Because of the complexity of the system under investigation, water pollution characterization is one of the most challenging tasks to confront the analytical chemist.

Design of measurement systems begins with defining (a) **WHY** the analysis is needed, (b) **WHAT** are the parameters to look for, and (c) **HOW** to perform the analysis. Water pollution measurement programs usually incorporate a multitude of physical, chemical and biochemical procedures. The characterization of physicochemical and biochemical transformations in aquatic environments takes into account interactions between atmosphere, hydrosphere and lithosphere and their influence on the aquatic habitat. Trace characterization of persistent organic residues or heavy metals is based on defining their distribution dynamics in the aquatic system, e.g., storage and release by bottom sediments and accumulation and tolerance by aquatic biota.

Recent trends in water pollution measurement rely heavily on advanced instrumental methods and automated analytical techniques. *In situ* sensor systems and remote noncontact optical measurement have been applied for monitoring water quality in rivers, lakes and waste effluents. The effects of environmental factors and interferences on the reliability of the measurement system have been under intensive research.

As America's water pollution problems become more complex, more complex measurement techniques are needed to cope with them. Above all, the effectiveness of pollution control programs are limited by their measurement reliability.

**SP354. Dental materials research.** Proceedings of the 50th Anniversary Symposium held at the National Bureau of Standards, Gaithersburg, Md., Oct. 6-8, 1969, in Recognition of Fifty Years of Dental Research at NBS, G. Dickson and J. M. Cassel, Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 354, 238 pages (July 1972).

**Key words:** Adhesives; composite restorative materials; dental materials research; dental restorative materials; future dental needs; laboratory testing and clinical research; mechanical properties; metals research; specifications.

A Symposium on Dental Materials Research was held at the National Bureau of Standards, October 6-8, 1969, on the occasion of the fiftieth anniversary of the dental research program at NBS. The Symposium brought together outstanding researchers in the dental materials field from throughout the world for a comprehensive examination of the present state of research and a

look at future dental needs and expectations. The program covered the broad dental materials field—from an examination of the oral environment to a consideration of future needs from the viewpoints of dental practice, dental education, dental industry, and basic science. Invited papers covered metals research, new developments in nonmetallic restorative materials, dynamic methods for determining the mechanical properties of dental materials, and problems of evaluating dental materials and making such evaluations useful to clinical dentistry through the development of specifications. *These proceedings include the following papers (indented):*

**Dental research at the National Bureau of Standards—reminiscences**, W. Souder, *SP354*, pp. 3-6 (July 1972).

**Key words:** Amalgam, dental; American Dental Association; dental materials; Dental Research Section, NBS; interferometer, dental; specifications, dental.

In 1918 dental amalgams had a high rate of failure and few data on their physical properties were available. Using the interferometer for determination of the dimensional changes of amalgam and scientific test methods of other properties, NBS began to obtain information on the physical properties of dental materials. The specification for dental amalgam developed in the early days with numerical limits for physical and clinical properties and details of test methods has served as a model for specifications for dental materials for over 40 years. Although the early results were challenged and the program opposed by some, the dental profession soon recognized the value of the work and requested its expansion. In time schools, dental associations, and manufacturers joined in commending the research program.

**Dental research at the National Bureau of Standards—history and individuals**, W. T. Sweeney, *SP354*, pp. 7-11 (July 1972).

**Key words:** Amalgam, dental; American Dental Association; casting, dental; dental research; Dental Research Section, NBS; guest workers; Paffenbarger, George C.; Schoonover, Irl C.; Souder, Wilmer; specifications, dental.

Dental research at NBS was initiated in 1919 by Dr. Wilmer Souder with work on dental amalgams. Dr. Souder built the Section on the principle of cooperation between research laboratories, manufacturers and the dental profession. In the 1920's research associates, first from the Weinstein Research Laboratory and later from the American Dental Association were added to the NBS dental research staff. Dr. N. O. Taylor and Dr. George C. Paffenbarger were the first ADA Research Associates. In 1945 while Dr. Irl C. Schoonover was Chief of the Section, the laboratory staff was further enlarged by the addition of Guest Workers from the Armed Services. Among the many important areas of research were precision casting, dental cements, polymers for dentures bases, composite restorative materials, high speed turbine handpieces, panoramic x-ray equipment, studies of natural tooth structure and development of standards and specifications.

**The need for basic research in dental materials**, F. A. Peyton, *SP354*, pp. 15-17 (July 1972).

**Key words:** Basic research related to dental materials; dental materials; interdisciplinary research; training of dental researchers.

The field of dental materials has benefited from basic studies of the silver-tin alloy system, of cobalt alloy systems, of polymers, and of many other areas. Future basic studies of the surface phenomena of wetting, spreading of liquid films, adhesion, diffusion into dental tissues, boundary interac-

tions, and principles of viscoelasticity related to dental materials offer productive opportunities. Basic research is essential if advances are to be made in the improvement, modification, refinement, and development of serviceable materials for the practice of dentistry. It is anticipated that such studies will increase in importance in the next quarter century and that basic scientists in many fields will be contributing to the improvement of dental service.

**Research needed by the Federal Dental Services, H. I. Copeland, *SP354*, pp. 19-21 (July 1972).**

**Key words:** Capabilities and needs of Federal Dental Services; dental research laboratories, Federal; dental staff; Federal Dental Services.

The dental research laboratories of the Federal Government function within the Departments of Commerce; Health, Education and Welfare; and Defense. These laboratories and the multidisciplinary scientists therein along with those of the Veterans Administration provide a much needed national resource. The Federal Dental Services have problems in common with each other and with the profession at large, in addition to having problems unique to themselves. Each Federal Dental Service needs a scientific staff capability to solve its own immediate problems or to contract for the solutions.

**Research needed by the dental industry, J. F. Glenn, *SP354*, pp. 23-26 (July 1972).**

**Key words:** Clinical and laboratory data correlation; dental industry research needs; dental materials; dental research, necessity for rapid communication of.

Dental industry requires new research information which must come from nonindustrial research-oriented institutions. Two major requests of dental industry are for basic research and better clinical correlation with laboratory data. Many compilations of physical test data on a variety of existing materials or ill-defined experimental ones are being reported, but the major need is for evaluation of these same materials in well controlled clinical applications. More rapid access to results of investigations, especially government-supported grant research, is needed.

**Research needed for dental education and practice, R. W. Phillips, *SP354*, pp. 27-30 (July 1972).**

**Key words:** Dental education; dental materials, research needs; dental practice future; dental research; materials, dental, research.

The current research effort in dentistry, and that which will occur during the next decade indicate that dental practice will be characterized by certain trends. These trends will require an acceleration of research on adhesive film forming systems, sealants for pit and fissures and means of improving anticariogenic characteristics of restorative materials. The interdisciplinary aspects of dental materials will be increasingly important. Greater focus will be on the biological properties of materials, materials and devices for oral rehabilitation, materials for implantation and the interaction of tissue and substances used to restore lost tooth structure. Further definition of the oral cavity can be expected to become a responsibility of the materials scientist. Increased emphasis can be expected in dental education on a more intimate basic science-clinical application orientation.

**Amalgams in dentistry, K. D. Jørgensen, *SP354*, pp. 33-41 (July 1972).**

**Key words:** Amalgam, dental; amalgam, dental, effect of technique on corrosion; clinical failure of amalgam; corrosion, dental amalgam; dental materials; marginal fracture, dental amalgam; mercurioscopic expansion, dental amalgam; porosity of dental amalgam.

Corrosion is a major factor in the failure of amalgam restorations through the deposition of corrosion products which may cause chronic periodontitis or through corrosion fracture of the margins which may cause secondary caries. Galvanic corrosion attacks only the tin-mercury  $\gamma_2$  phase. Mercury released by this corrosion causes a mercurioscopic expansion resulting in a deflection of the amalgam from the cavity wall at the margin. Corrosion can be considerably reduced by minimizing the porosity of the amalgam restoration through overfilling the cavity, burnishing the margins, eliminating excess by carving and using zinc-containing amalgams.

**Basic metallurgy of dental amalgam, L. B. Johnson, Jr., and H. G. F. Wilsdorf, *SP354*, pp. 43-59 (July 1972).**

**Key words:** Amalgam, dental; amalgam, metallurgy; amalgam, strength; corrosion of dental amalgam; dental materials; metallurgy of dental amalgam.

An "equilibrium" mixture of components of dental amalgam would contain the phases  $\beta_1$ ,  $\gamma_1$  and  $\gamma_2$  shown by Gaylor. Because dental amalgam is formed clinically at relatively low temperature only  $\gamma_1$  and  $\gamma_2$  are generally found. The tensile strengths of the Ag-Hg and the Sn-Hg matrix phases of dental amalgam are considerably below the tensile strength of the amalgam while the tensile strength of  $\text{Ag}_3\text{Sn}$  is considerably above that of the amalgam. Cleaning the alloy powder with 5 percent HCl promotes better bonding between matrix and  $\text{Ag}_3\text{Sn}$  and significantly increases the tensile strength. The  $\gamma_2$  phase of amalgam is the only phase subject to destructive corrosion. The  $\gamma_2$  phase has been successfully eliminated from amalgam by two methods: (1) by inclusion of powder consisting of the Ag-Cu eutectic in the alloy and (2) by substitution of 10 percent Au for Ag in the alloy.

**Casting alloys in dentistry, K. Asgar, *SP354*, pp. 61-66 (July 1972).**

**Key words:** Castings, dental, accuracy; castings, lost wax technique; dental materials; gold alloys, dental; high heat casting technique; hygroscopic expansion; investment, dental; thermal expansion casting technique; wax, inlay casting.

A major difference between the two techniques, hygroscopic and high heat or thermal expansion, used for casting gold alloys is that the wax pattern can offer some resistance to hygroscopic expansion of the mold while it does not resist thermal expansion. Researchers have condemned the hygroscopic technique because of nonuniform expansion of the wax pattern but have not given sufficient attention to other nonuniform dimensional changes which are present in both techniques and which may combine to affect favorably or unfavorably the accuracy and retention of the casting. Studies in this field should not be limited to simple measurements of thermal, setting and hygroscopic expansions of the investment but should be expanded to include strength of the investment along with its roughness, strength and behavior of waxes, and shrinkage patterns of molten metals. A need for new types of investments is presented by the recent development of many new nonprecious alloys for dental castings.



**Basic metallurgy of dental casting alloys**, J. P. Nielsen, *SP354*, pp. 67-73 (July 1972).

**Key words:** Alloys, dental casting; ceramic-metal systems; chrome-cobalt alloys; dental materials; gold alloys; metallurgy, dental alloy; porcelain-gold materials; solder, gold alloy.

The complex dental casting alloys have arrived at their present useful state mostly by trial and error. The three areas of technical significance for these alloys are: inertness in the oral environment, fabricability (including soldering), and alloy strengthening. Basic metallurgical studies are being made in this area, and as the gap between the art and basic metallurgy is closed, improvement in properties and the cutting down of precious metal content can be expected. There are prospects of new alloy systems and improvement in casting technique, particularly in automatic casting. Ceramic metal systems need further study. For the long range, investigations of the prosthetic material-human tissue reactions are necessary. To assist studies in this field a dental materials handbook on properties of dental alloys and related materials should be compiled and published.

**Dental porcelain**, J. W. McLean, *SP354*, pp. 77-83 (July 1972).

**Key words:** Aluminous porcelain; ceramic materials, dental; dental materials; dental porcelain; dispersion strengthening of glass; porcelain, dental; porcelain-gold techniques and materials.

Current research on dental porcelain has been concentrated on methods of improving fracture resistance of porcelain restorations. Enamelling of metals or dispersion strengthening of glasses offer the greatest possibilities for this purpose. The fusion of porcelain to metal copings has proved very successful under clinical conditions, but the necessity for masking the metal substructure presents difficulties in obtaining the desired aesthetic characteristics. Replacement of the metal copings by a higher strength ceramic should improve aesthetics and reduce productive costs. Dispersion strengthening of glass with high strength alumina crystals has resulted in the production of a new range of aluminous porcelains for jacket crown and bridge pontic construction.

**Dental silicate cements**, A. D. Wilson, *SP354*, pp. 85-92 (July 1972).

**Key words:** Aluminum phosphate, amorphous; dental materials; dental silicate cements; electron probe microanalysis; glass, aluminosilicate; silica gel; silicate cements, dental; silicate cements, mechanism of hardening, microstructure of, chemical nature; silicate cements, susceptibility to acid attack.

A systematic search for improvement of dental silicate cements requires detailed knowledge of their formation and structure. Experimental evidence shows the effective bonding medium in these cements is an amorphous aluminum phosphate. Physicochemical examination of a number of dental silicate powders showed them to be powdered fluorine-containing aluminosilicate glasses. The mechanism of the cement-forming reaction was studied for one cement following extraction of soluble ions by water at various time intervals after preparation. Infrared spectroscopy was used to record the changing absorption spectra of the setting cement. The microstructure of a number of fully hardened cements was studied by a variety of techniques: optical and electron microscopy, electron probe microanalysis infrared spectroscopy and x-ray diffraction. Dissolution in acidic

media of aluminum phosphate bonded silicate cements is an inherent defect stemming from the fundamental chemistry of the system.

**Composite restorative materials**, R. L. Bowen, J. A. Barton, Jr., and A. L. Mullineaux, *SP354*, pp. 93-100 (July 1972).

**Key words:** Biomaterials; composites; dentistry; fillers; glass; methacrylates; monomers; prostheses; resins; restorative material.

This article describes the development of dental composite materials, which have quickly established a place in the practice of dentistry because of the shortcomings of alternative esthetic direct filling materials. The goal-directed basic research in which the composite materials were developed was initiated at the National Bureau of Standards in 1956. Late in 1957, a monomer was synthesized that is suitable for use with reinforcing fillers. Commercial dental composite materials available in 1969 use this resin together with particulate fillers and various additives; they have lower polymerization shrinkage and coefficient of thermal expansion, and higher compressive strength and stiffness relative to unreinforced resins. Compared to silicate cements, the composites have lower solubility, higher tensile strength, and comparable compressive strength. Composite restorative materials, when they have been fully developed, should provide the dental profession and the public with greatly improved restorations for anterior teeth.

**Cements containing *o*-ethoxybenzoic acid (EBA)**, G. M. Brauer, *SP354*, pp. 101-111 (July 1972).

**Key words:** Crown and bridge cements; dental cements; EBA cements; EBA sedative bases; intermediate restorative; *o*-ethoxybenzoic acid cements; pulp capping materials; zinc oxide-EBA-eugenol cements.

Cements containing *o*-ethoxybenzoic acid (EBA) are reviewed. Studies of the mechanism of hardening of zinc oxide-eugenol cements indicated the potential usefulness of other chelating agents in dental cements. Products with greatly enhanced physical and mechanical properties are obtained by the partial substitution of EBA for eugenol. Similar to zinc oxide-eugenol cements, these materials are well tolerated by the tissues, but they also stimulate the formation of reparative dentin. Physical properties of the EBA-containing cements approach those of the biologically and physiologically less desirable zinc phosphate cements. The EBA cements have become commercially available and have been well accepted as luting agents for fixed restorations and as insulating bases. They appear to be the materials of choice for indirect pulp capping. Resin modified EBA restoratives show good stress-bearing characteristics and should find applications as an intermediate restorative. Possible studies to further improve these versatile materials are discussed.

**Organic adhesives**, H. Alter and A. Fookson, *SP354*, pp. 113-123 (July 1972).

**Key words:** Critical surface tension; dental adhesion improvement through liners, coupling agents, fillers, and surface treatment; dental adhesives to include acrylates, cyanoacrylates, epoxy resins and polyurethanes; dental materials; polyurethane.

The materials and means for improving joint strengths in a wet environment between dentin or enamel and restoration or cavity liner are reviewed. Critical surface tension,  $\gamma_c$ , a descriptive property of surfaces, offers a basis to evaluate capacity of adhesives to wet tooth surfaces. Used as a

pretreatment, an adhesive may function by displacing water. Attachment to tooth surface through hydrogen bonding may also occur. Adhesion may be improved by use of liners, coupling agents, fillers and tooth surface treatments such as etching processes. Dental adhesive materials include acrylics, cyanoacrylates, epoxy resins and polyurethanes, the latter having apparently good promise as a dental adhesive of the future.

**Viscoelastic behavior**, P. L. Oglesby, *SP354*, pp. 127-144 (July 1972).

**Key words:** Amalgam, dental; creep; dental materials; denture base resins; indentation test method; mechanical properties, dental materials; rocking beam oscillator; stress relaxation; torsion pendulum; viscoelastic methods.

Since the mechanical responses of many dental materials are functions of time as well as of applied stress, viscoelastic theory, and experimental methods should be used in describing and characterizing these materials. Both static and dynamic methods may be used. Viscoelastic theory useful for characterization of dental materials and for interrelation of responses under different types of static and dynamic tests includes the Boltzmann superposition principle for linear materials and as modified and extended for non-linear materials, the time-temperature superposition principle and approximation methods for calculation of relaxation and retardation spectra. Methods which have been applied to dental materials such as amalgam, polymeric restorative materials, elastic impression materials and natural tooth structure include creep, stress relaxation, indentation and forced vibration methods.

**Low frequency determination of mechanical properties**, R. L. Myerson, *SP354*, pp. 145-160 (July 1972).

**Key words:** Activation energy; dental materials; glass, sodium phosphate; internal friction; mechanical properties; polymers, dental; torsion pendulum.

The torsion pendulum is a valuable tool for use in determining the mechanical properties and molecular structure of dental materials. With the torsion pendulum the modulus of a material may be determined from the frequency of oscillation; the internal friction can be obtained from the rate of damping. Change in internal friction with change in frequency provides insight into type of structure and relaxation mechanisms. Activation energy of processes can be determined from shift in peak energy absorption temperature with change in frequency. A principal advantage of low frequency testing is in the resolution of dispersions or of internal friction peaks. The torsion pendulum method has been applied to various polymer materials in studies of the relationship of composition and transitions, effects of cross-linking, comparison of cast poly(methyl methacrylate) and powder-liquid molded poly(methyl methacrylate) and the relationship of impact resistance to peak energy absorption temperatures. Studies have been made of the relationships between peak temperatures and composition and cross-linking in sodium phosphate glasses. A review of equipment is presented.

**Ultrasonic methods for determination of mechanical properties**, G. Dickson, *SP354*, pp. 161-168 (July 1972).

**Key words:** Dental amalgam; dental materials; elastic properties; mechanical properties; nondestructive testing; ultrasonic techniques.

Elastic characteristics, shear modulus, Young's modulus, bulk modulus and Poisson's ratio for materials can be deter-

mined by a variety of ultrasonic methods, most of which involve the measurement of the velocity of sound in the material. The methods are precise, rapid, nondestructive and applicable to small specimens. As a number of reports in the literature indicate, ultrasonic methods offer particular advantages to the study of dental materials and mineralized tissues.

**Stress analysis of dental structures**, R. G. Craig, *SP354*, pp. 169-175 (July 1972).

**Key words:** Brittle coatings for stress analysis; dental materials; denture, artificial, stress analysis; photoelasticity, dental applications; porcelain-gold restorations, stress analysis; stress analysis of dental structures.

Because of the complex geometry of dental structures, most stress analysis studies in dentistry have been experimental. Brittle coatings have provided generally semiquantitative information on the magnitude, direction and sign of surface stress of fixed bridges, removable partial dentures, complete dentures and the mandible under various loading conditions. Data from electrical resistance strain gages attached to the metal surfaces of pontics on a gold bridge with various load applications are shown. Applications of both two and three dimensional photoelastic techniques are illustrated. This method, which provides information on the magnitude, direction and sign of boundary and internal stresses is dependent upon how well the model represents the real structure. Other stress analysis methods involve photoelastic coatings, thermophotoelasticity, moire fringe patterns, holography and x-ray diffraction.

**Relations between mechanical properties and clinical behavior**, D. B. Mahler, *SP354*, pp. 177-180 (July 1972).

**Key words:** Amalgam, dental; correlation of laboratory and clinical evaluations; creep of dental amalgam; dental materials; dynamic creep; fracture, marginal of dental amalgam; mechanical properties of dental materials; rheological properties of dental amalgam.

A dilemma in the field of dental materials is that in many instances the critical physical properties that are relevant to the failure of restorative materials have not been identified or when identified the limiting values which separate successful from unsuccessful materials have not been established. To determine the critical property relevant to clinical marginal fracture of dental amalgam restorations, dynamic creep and other physical properties including compressive, tensile and transverse strength and transverse deflection of nine amalgam alloys were determined. Clinical evaluation of restorations made using alloys widely separated in dynamic creep showed that marginal fracture was associated with the rheological properties of dynamic creep, static creep and slow compressive strength, but showed little relationship to the other physical properties measured. Although the relationship between creep and marginal fracture may not be a cause and effect mechanism, creep appears to be reasonably predictive of clinical marginal fracture.

**Need for research to develop performance characteristics**, H. P. L. Schoenmakers, *SP354*, pp. 183-186 (July 1972).

**Key words:** Clinically related strength properties of dental materials; dental materials; dental materials, correlation of bulk and marginal properties; dental materials, performance characteristics; dental restorations, the role of oral environment factors in stability thereof.

To develop the most important characteristics of restorative materials, an understanding of the processes by which



margins of such restorations become damaged is needed. Bulk and margin properties should be correlated. The mechanical forces developed in mastication and chemical attack by the oral environment are important factors. Tensile strength appears a more meaningful data than either shear or compressive strength. Research for selection of proper tensile test procedures is needed. Cracks and voids in specimens complicate their strength behavior. The role of temperature in laboratory evaluation is important. The mechanisms of corrosion and erosion of dental restorations require further research.

**Need for correlation between laboratory testing and clinical research,** B. Hedegård, *SP354*, pp. 187-189 (July 1972).

**Key words:** Aging processes, relation to dentistry; clinical research, dental; correlation of laboratory and clinical results; dental materials; dentistry, preventative; dentistry, restorative; epidemiological information, dental.

Although priority must be given to basic and clinical research in preventive dentistry, this does not eliminate the need for research on materials and methods for restorative dentistry which is in itself a preventive measure. There is an urgent need for collaborative and correlative studies involving properties of materials to be studied in the laboratory and tested in the clinic. Clinical research with materials is slow, and with the present incomplete information on oral environment and function, it is often difficult to assess properly the results, but there is no alternative. With sound clinical research on a larger and more penetrating scale, data and information may be obtained that will make it possible to set up more meaningful test procedures in the laboratory. And that is the goal: to be able to characterize the dental material in the laboratory and correctly predict its clinical performance.

**Biological evaluation of dental materials,** G. Ryge, *SP354*, pp. 191-200 (July 1972).

**Key words:** Biological evaluation of dental materials; clinical evaluation of dental materials; correlation of laboratory and clinical performance; dental materials; restorative materials; toxicity tests.

Biological evaluation of dental materials includes (1) screening for toxic or other untoward effects of the materials, and (2) clinical evaluation of materials that pass the screening tests. Screening tests must take into account the functional requirements of various types of and service conditions for dental and auxiliary materials. Methodology for evaluation of clinical performance of materials must include examiner training and calibration in the use of rating scales. Emphasis is placed on the need for correlation of laboratory properties with clinical performance.

**Corrosion testing in the mouth,** K. Nagai, *SP354*, pp. 201-205 (July 1972).

**Key words:** Base-metal alloys, dental; copper-zinc dental alloy; corrosion, clinical tests; corrosion of dental alloys; dental amalgam; dental materials.

For many years various base-metal alloys were used as substitutes for gold alloys for dental restorations in Japan. The adoption of an official requirement that these alloys should not have a weight loss of more than 3 mg/cm<sup>2</sup> when immersed in solutions of 0.05 percent hydrochloric acid, 1 percent lactic acid, 1 percent sodium chloride, and 0.1 percent sodium sulfide for three days, prompted a study of corrosion of a copper-zinc alloy and dental amalgam in the mouth. Cast copper-zinc specimens had average weight

losses in the mouth in the range of 0.022 to 0.034 mg/cm<sup>2</sup> per day. Conventional amalgams had losses as small as 0.0063 mg/cm<sup>2</sup> per day. Weight losses in the test solutions ranged up to 150 times those in the mouth while weight losses in artificial saliva in vitro were about twice those in the mouth. It is believed that the lower corrosion in the mouth (which varies from place to place) results from a cleaning and inhibiting action by the saliva.

**International specification program—Australian experience,** A. R. Docking, *SP354*, pp. 209-211 (July 1972).

**Key words:** Accreditation of dental materials, Australian experience; Australian dental specifications; dental materials; dental standards; specifications, dental.

The Australian dental specifications as a basis for a certification program were developed through the Standards Association of Australia and not within the dental association. Products are accredited by the Australian Dental Association on the basis of meeting these specification tests. The Commonwealth Bureau of Dental Standards assists in preparation of specifications and in accreditation of products. Approximately thirty Australian dental standards have been issued. Participation in international specification work has proved of great benefit especially in the raising and maintenance of the quality of dental goods used by the Australian dental profession.

**Development of European specifications and testing,** P. Laplaud, *SP354*, pp. 213-215 (July 1972).

**Key words:** Certification; dental specification; European dental specifications; FDI; ISO; terminology, dental.

The development of a European specification program is difficult because of the many differences of race, nationality, politics, and social systems. One of the first problems is the establishment of a common dental terminology. The lack of sufficient data on the relationship of properties and clinical results is another difficulty. However, Europe has a long heritage of standardization in other fields and this has made it logical to think of the ISO as the proper organization to introduce international dental standards into Europe. Many European countries have already achieved promising results on a national basis. Cooperation on a regional or continental level in the development of a specification and certification program will help to provide better dental health for the public.

**Development of South American specifications and testing—Brazilian experience,** L. W. Süffert, *SP354*, pp. 217-220 (July 1972).

**Key words:** Brazilian experience, dental materials specifications; dental materials; dental specifications; dental specifications and testing, South American.

A successful program of specifications for dental materials requires extensive knowledge of and participation in the program on the part of teachers in dental schools. In turn the dental teachers can involve dental industry and dental societies. In Brazil a specifications program in dental materials was initiated by holding annual meetings to which persons recognized as authorities in dental materials were invited to lecture and give assistance in specification aspects. Certification testing of dental materials has been initiated in only two dental schools, but it is planned to have dental materials departments at selected dental schools responsible for three or four materials in a general certification testing program.

**USA specification and evaluation programs,** J. W. Stanford, *SP354*, pp. 221-224 (July 1972).

Key words: Dental materials and devices, specifications for and certification of; dental specifications; specifications; standards, dental.

Reliable and valid laboratory tests which delineate satisfactory materials and rule out unsatisfactory ones are essential to the development of a satisfactory specifications program. Factors guiding the American Dental Association in the formulation of specifications are: Relevant tests; correlation of laboratory, structural, and service tests; and quality of product. An important change in organization for the development of dental specifications involves the formation of the USA Standards Committee for Dentistry, operating under the United States of America Standards Institute. The Certification Program provides a means for recognition of those materials complying with existing specifications. A new evaluation program on dental devices is currently issuing pertinent status reports on the safety and efficiency of such devices. Safety and usefulness are based primarily upon information established under conditions of clinical use.

**SP356. Damage in laser materials: 1971.** Proceedings of a symposium sponsored by the American Society for Testing and Materials and by the National Bureau of Standards, May 19-20, 1971, NBS, Boulder, Colo., A. J. Glass and A. H. Guenther, Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 356, 174 pages (Nov. 1971).

Key words: Laser damage; laser materials; self-focusing.

The third ASTM Symposium on Damage in Laser Materials was held at the National Bureau of Standards in Boulder, Colo., on May 19-20 of this year. The symposium is held as part of the activity of Subcommittee II on Lasers and Laser Materials, of the ASTM. Subcommittee II is charged with the responsibility of formulating standards for laser materials, components, and devices. The chairman of Subcommittee II is John D. Myers, of Owens-Illinois, Inc. Co-chairmen for the damage symposia are Dr. Arthur H. Guenther, of the Air Force Weapons Laboratory, and Professor Alexander J. Glass, Chairman of the Department of Electrical Engineering at Wayne State University.

Approximately 50 attendees at the symposium heard 17 papers on topics relating to laser-induced damage in glass, crystalline materials, nonlinear optical materials, thin film dielectric coatings, and mirrors. Particular attention was given to the processes of plasma formation at dielectric surfaces, and to the role played by self-focusing in bulk damage in solids. The principal recommendations for future investigations are summarized below.

The proceedings of these Symposia represent the major source of information in the field of damage in laser materials. The Symposia themselves, along with the periodic meetings of Subcommittee II, provide a unique forum for the exchange of information regarding laser materials specifications among the manufacturers and users of laser devices, components and systems. The symposium also serves as a mechanism of information gathering, to enable the Subcommittee to write informed and realistic specifications.

**SP357. The mechanisms of pyrolysis, oxidation, and burning of organic materials.** Based on Invited Papers and Discussion, 4th Materials Research Symposium held at the National Bureau of Standards, Gaithersburg, Md., Oct. 26-29, 1970, L. A. Wall, Editor, Nat. Bur. Stand. (U.S.), Spec. Publ. 357, 199 pages (June 1972).

Key words: Burning; hydrocarbons; organic materials; oxidation; polymers; pyrolysis.

A symposium on The Mechanisms of Pyrolysis, Oxidation, and Burning of Organic Materials was held at the National Bureau of Standards in October 1970. This volume contains the nineteen papers presented and much of the discussion which followed.

These papers review and discuss the current status of kinetic studies on the reactions of organic materials in both gas and condensed phases. The topics covered include: pyrolysis of hydrocarbons, pyrolysis of polymers, oxidation of polymers, oxidation of organic compounds, burning of organic compounds and burning of polymers. Particular emphasis is placed on the elucidation of the mechanisms of reaction in terms of free radicals or other transient species and physical effects. *These proceedings include the following papers (indented):*

**The genesis of free radical chemistry,** F. O. Rice, *SP357*, pp. 1-6 (June 1972).

Key words: Alchemy; free radicals; genesis; phlogiston; valency.

Modern chemistry is a late-comer among the sciences and came into being only at the beginning of the 19th century when the phlogiston theory was abandoned to be replaced by Dalton's Atomic Theory. As Dalton's Theory became firmly established, there grew with it the belief known as the doctrine of valency which resulted, by the middle of the 19th century, in the denial of the very existence of free radicals.

In the early 20th century, the work of many scientists—Hinshelwood, Bodenstein, Taylor—in the fields of photochemistry and kinetics led to the belief that free radicals not only existed but played an important part in the mechanism of chemical transformations. Paneth's discovery that free radicals could be detected by their removal of certain metallic mirrors was followed by Rice's demonstration that organic compounds did decompose thermally into free radicals and then the Rice-Herzfeld theory that showed it was possible to explain quantitatively the mechanism of the thermal decomposition of organic compounds. In *The Annual Review of Physical Chemistry* (1971), a chapter on Paraffin Pyrolysis contains the following sentence: "All in this field are not agreed that the reactions can basically be described in terms of the Rice-Herzfeld radical chain mechanisms and that, in general, chains are long."

**Pyrolysis of organic compounds in the gas phase,** A. S. Gordon and R. H. Knipe, *SP357*, pp. 7-15 (June 1972).

Key words: Decomposition; kinetics of decomposition; molecular mechanisms; pyrolysis of hydrocarbons; radical mechanisms; unimolecular decomposition.

A critical review of the pyrolysis of organic compounds is made. The review is divided into hydrocarbons, halides, and oxy compounds. Most hydrocarbon reactions have an important unimolecular component, either the initial step in the case of chain reactions (e.g., saturated hydrocarbon decomposition) or a one-step reaction which may involve a transient biradical structure. There are many types of pyrolysis reactions in the latter category.

For halocarbon pyrolysis, there are two reaction paths, one involving a unimolecular rupture of the carbon-halogen bond and the other a unimolecular elimination of the hydrogen halide molecule via a polarized activated complex. The preferred path is determined by the self-quenching efficiency of the radical path. If highly efficient, the molecular elimination path will dominate and vice versa. In some systems, the two paths are competitive.

Oxy hydrocarbons such as acids and esters pyrolyze via the polarized complex molecular elimination path. Ethers



appear to pyrolyze via a free radical chain mechanism while ethylene oxide is initiated by a unimolecular rearrangement to acetaldehyde with excess energy. The vibrationally excited molecule can decompose into two radicals and initiate chain decomposition.

**Pyrolysis of hydrocarbons**, M. H. Back, *SP357*, pp. 17-25 (June 1972).

**Key words:** Acetylene; dissociation; elementary reactions; ethane; ethylene; hydrocarbons; kinetics; mechanism; methane; olefins; paraffins; propylene; pyrolysis; rate constants; unimolecular theory.

Some current problems arising from studies of the pyrolysis of hydrocarbons are discussed and two stages of these studies are distinguished. The first stage concerns the description of the mechanism of the pyrolysis in terms of a series of elementary reactions. The types of reactions occurring during the pyrolysis of olefins are discussed from this point of view and the effects of temperature and pressure on these elementary reactions are shown to produce predictable changes in the overall pyrolysis. Some problems in the mechanism for the pyrolysis of acetylene are discussed and a mechanism proposed which relates the reactions occurring in both the high and low temperature regions. The second stage in pyrolysis studies is attained when the mechanism of the reaction may be satisfactorily described in detail and experiments may then be designed to measure the rate constants of the elementary processes. Several studies on the paraffins have attained this goal and the results are examined for consistency with related measurements.

**Factors involved in the degradation of polymers in melts**, C. R. Patrick, *SP357*, pp. 33-43 (June 1972).

**Key words:** Degradation of polymers in melts; diffusion-controlled reactions between macroradicals; diffusivities of molecules and radicals in molten polymers; geminate recombination of radicals; pyrolysis of hydrocarbons; rates of reaction in liquids and gases; reaction equilibria in liquids and gases.

The full interpretation of degradation of molten polymer would be facilitated by a better understanding of the elementary chemical processes involved. Suitable analogs of these reactions may often be studied in detail only in the gas phase. Relationships between the kinetics of elementary reactions in gas and liquid phases are desirable. On the basis of thermodynamic arguments, it is concluded that Arrhenius parameters for bimolecular reactions in the two phases should differ, to a small but significant extent, greater than usually accepted, whilst those for unimolecular processes, commonly should not. Diffusion may determine the rates of some reactions in liquids particularly of reactions between radicals. Evidence on the mobilities of large and small molecules, models for radicals, in molten polymers, is summarized. Expressions for diffusion-controlled reactions are compared and applied to reactions in molten polymers. Complicating effects in the size dependence of the rates of diffusion-controlled reactions between macroradicals are surveyed. Other complicating effects, notably of geminate reactions between radicals, are discussed. A case is made out for comparing more extensively the kinetics of thermal degradation of gaseous paraffins, and of molten paraffins and polyethylenes.

**Pyrolysis of polymers**, L. A. Wall, *SP357*, pp. 47-60 (June 1972).

**Key words:** Chain scission; crosslinking; polymers; pyrolysis; stripping.

The nature of their pyrolysis products, monomer, oligomers and carbonaceous residues enables one to group polymers into three classes, those that decompose by net main chain scission; by stripping of the main chain, for example the thermal dehydrochlorination of polyvinyl chloride; and by crosslinking of the main chain followed by some production of volatiles. Highly unsaturated or aromatic chains tend to follow the latter course.

At the present time, a theoretical framework exists which permits, provided adequate experiments are performed, the elucidation of the decompositions of the first type. For most of the well-known polymers in this class, this framework of knowledge gives very acceptable mechanistic explanations or interpretations of the decomposition process based on observations of rate of weight loss, of molecular weight changes and composition of volatile products.

Knowledge of the decomposition of the second class of polymers is at an intermediate state of development. However, an important practical research objective would be the acquisition of methods for converting the mechanisms of decomposition of class one substances to that for class two type.

For the third class of materials, knowledge of their pyrolysis mechanisms is nonexistent. This is largely due to the fact that methods for quantitatively following solid-phase processes of decomposition are relatively difficult and unsatisfactory.

**Patterns and problems in the pyrolysis behaviour of synthetic addition polymers**, G. G. Cameron, *SP357*, pp. 61-70 (June 1972).

**Key words:** Free radicals; polymer abnormalities; polymer degradation; polymer pyrolysis; transfer reactions.

The types of pyrolytic decomposition reactions undergone by synthetic addition polymers are outlined. Particular attention is given to two classes of polymer—those which undergo unzipping to monomer and those which fragment randomly along the backbone to yield low polymer. Free radical transfer reactions, usually involving tertiary hydrogen atoms, can play an important part in these degradation reactions. The thermal stability of addition polymers is not always predictable from known reactions of small molecules. This is often due to the presence of labile irregularities which are chemically incorporated in the macromolecules and which can initiate thermal decomposition. Also, since polymers are susceptible to chain reactions and neighbouring group effects, these abnormalities can affect the stability of a large proportion of the sample. The effects on pyrolysis of abnormalities such as unsaturation, chain branches, head-to-head links and oxidation products are discussed.

**On certain problems connected with the inhibited oxidation theory**, Yu. A. Shlyapnikov, *SP357*, pp. 73-78 (June 1972).

**Key words:** Antioxidants; inhibition of oxidation; initiation of oxidation; oxidation mechanism; oxidation theory.

The oxidative reactions of organic compounds and polymers are discussed in terms of free radical mechanisms, with particular emphasis on initiation, inhibition, and stabilization phenomena.

**Mechanism of peroxydation of polymers**, A. Chapiro, *SP357*, pp. 79-82 (June 1972).

**Key words:** Hydroperoxides versus diperoxides; influence of polymer phase on peroxidation; influence of temperature on peroxidation; peroxidation of polyethylene; peroxidation of polymers; peroxidation of polypropylene; peroxidation of poly(vinyl chloride).

The irradiation of polymers in the presence of air leads to polymeric hydroperoxides POOH and diperoxides POOP. When such irradiated polymers are used to initiate the polymerization of a monomer, hydroperoxides generate equal amounts of graft copolymer and homopolymer, whereas diperoxides only generate graft copolymer. This technique was used to study the peroxidation of various polymers under different irradiation conditions. It was found that polypropylene irradiated at temperatures ranging from 10 to 60 °C undergoes hydroperoxidation by a chain reaction. At 0 °C and below (in the vitreous polymer) polymeric radicals are formed but remain trapped. Poly(vinyl chloride) also leads to hydroperoxides when irradiated at 20 to 60 °C but no chain process develops below the glass transition temperature. Irradiation of the plasticized polymer leads to a hydroperoxidation by a short chain mechanism. It is concluded that the propagation of the hydroperoxidation chain, involving hydrogen abstraction by PO<sub>2</sub> radicals, only occurs above *T<sub>g</sub>* when the mobility of polymeric segments is sufficient to ensure the interaction of PO<sub>2</sub> with neighboring molecules.

Polyethylene irradiated at room temperature chiefly generates diperoxides POOP. The chain hydroperoxidation only sets in above 35 °C. Below this temperature, recombination of PO<sub>2</sub> radicals occurs faster than hydrogen abstraction. The behaviour of polymers with respect to peroxidation is discussed and compared with that of low molecular weight model compounds.

**Oxidative degradation of polymers and organic compounds via unimolecular decomposition of peroxy radicals**, J. Marchal, *SP357*, pp. 85-92 (June 1972).

**Key words:** Kinetics; mechanism; organic compound; oxidative degradation; peroxy radical isomerization; poly(ethylene oxide); polymer; polypropylene; poly(propylene oxide); polystyrene; polytetrahydrofuran; room temperature; 1,4-dioxane.

Autoxidation of various polymers and organic compounds is shown to include, already at room temperature, chain scissions involving unimolecular decomposition of secondary and tertiary peroxy radicals. Rate and product data are consistent with a scheme including a six-membered ring transition state leading to three fragments, one of them being an alkoxy radical. This oxidative degradation scheme at room temperature does not correspond to a known mechanism.

**Mechanisms of oxidation of polyolefins below 150 °C**, F. R. Mayo, *SP357*, pp. 95-98 (June 1972).

**Key words:** Alkoxy radicals; carbonyl compounds; chain initiation; chain propagation; chain termination; kinetics; oxidation; peroxy radicals; polyolefins; polypropylene.

This paper applies what we have learned about oxidations of simple aliphatic hydrocarbons below 150 °C to oxidations of bulk polyolefins. The principal difference between these groups is due to the production of initiating radicals in pairs and to the greatly restricted mobilities of all radicals. Data are given for the efficiency of initiation by di-*t*-butylperoxy oxalate of the oxidation of atactic polypropylene at 45 °C and for the effect of peroxide concentration on efficiency and kinetic chain length. The following other topics are discussed: chain propagation and geminate and statistical termination by alkylperoxy radicals, nonterminating reactions of two tertiary alkoxy radicals, formation and reactions of alkoxy radicals, sensitivity of oxidation products to further oxidation, intramolecular propagation of alkylperoxy radicals, and the question of the formation of carbonyl groups in oxidations of polyolefins.

**Polymer-gas reactions (air pollutants: NO<sub>2</sub> and SO<sub>2</sub>) as function of pressure, UV light, temperature, and morphology – a survey**, H. H. G. Jellinek, *SP357*, pp. 101-109 (June 1972).

**Key words:** Air pollutants; butylrubber, degradation, effect of NO<sub>2</sub>; degradation, effect of morphology; effect on polymers of NO<sub>2</sub>, SO<sub>2</sub>, air and UV light; nylon, degradation, effect of NO<sub>2</sub>; polymer-gas reactions; polystyrene, atactic, degradation, effect of NO<sub>2</sub>; polystyrene, diffusion of NO<sub>2</sub> and degradation; polystyrene, isotactic, degradation, effect of SO<sub>2</sub>.

Reactions of various polymers, such as polystyrene and its stereo-specific isomers, butylrubber, nylon, etc., with nitrogen dioxide and sulfur-dioxide were studied by the author and co-workers in recent years. Mechanisms of these reactions in presence of these gases, near ultraviolet light and oxygen were elucidated. Diffusion phenomena have also been investigated and their importance has been pointed out. More recently, work has been initiated on the influence of polymer morphology on degradation of polymers in presence of these gases, near UV radiation and oxygen. Unexpected effects have been observed during chain scission near room temperature. Thus, for instance, isotactic polystyrene of various crystallinities, as far as extent and type are concerned, show marked differences in their degradation characteristics. Thus, for instance, crystalline polymers show faster degradation than amorphous ones, which seems to be contrary to expectations. However, this phenomenon can be explained in quite a consistent manner. The importance of all these reactions in connection with air pollution is briefly discussed.

**Controlled gaseous oxidations of organic compounds**, C. F. Cullis, *SP357*, pp. 111-117 (June 1972).

**Key words:** Concurrent reactions; consecutive reactions; controlled oxidation; conventional additive experiments; cool-flames; intermediate products; isobutane; isotopic tracer techniques; isotopically-labelled additives; macroscopic stages; mutual influences; *n*-butane; *n*-heptane; O-heterocycles; radio gas chromatographic analysis; selective inhibition; selectivity; self-inhibition; thermal control; 1-butene; 2-butene.

The homogeneous gaseous oxidation of organic compounds generally leads to a wide variety of products and this may be ascribed not only to the occurrence of a number of consecutive and concurrent reactions but also to the fact that the various constituent elementary steps tend to interact with one another in complex ways. Several methods are outlined for minimizing the extent of unwanted consecutive reactions but it appears to be much more difficult to restrict undesirable concurrent reactions. If the mutual influences of the various part-reactions are to be understood and controlled, it is important to elucidate the nature and role of the intermediate molecular products. Although here carefully planned experiments involving the artificial addition of reactive intermediates can yield some information, a much fuller understanding of the quantitative importance of the different competing reaction paths can be obtained from experiments with isotopically-labelled intermediates. Several examples are given of the use of isotopic tracer techniques in the unravelling of the mechanism of complex gaseous oxidation reactions.

**Some current problems in oxidation kinetics**, S. W. Benson, *SP357*, pp. 121-129 (June 1972).

**Key words:** Acetylene reaction with O<sub>3</sub>; activation energy for oxidation; chain lengths in oxidation; elementary steps



in oxidation; epoxidation; gas-phase oxidation; kinetics; liquid-phase oxidation; mechanism;  $O_3$  addition to unsaturated; oxetane formation in oxidation; oxidation; peroxy radicals; radical isomerization; surface effects in oxidation; termination rates; transition state for termination.

Experimental data on low temperature ( $< 150^\circ C$ ) and high temperature ( $> 250^\circ C$ ) oxidations are examined from the point of view of reported quantitative inconsistencies. Activation energies for  $tBuO_2$  metathesis reactions with alkanes appear to be 7 kcal/mole higher than for comparable reactions of  $HO_2$ . Related isomerization reactions are examined in the light of these differences without reaching any simple conclusions. The Russell mechanism for a 6-membered, cyclic, transition state for termination of primary and secondary alkyl peroxy radicals is shown to be either inconsistent with thermochemical data, or else unique to solution reactions. Addition reactions of  $O_3$  with olefins and acetylenes are shown thermochemically to have the possibility of following concerted and biradical pathways, respectively.

Recent data showing strong inhibition by  $PbO$ -coated surfaces of both oxidation and pyrolysis of  $i-C_4H_{10}$  are examined in terms of mechanism.

**Kinetics and mechanisms of flames and flame suppression, R. M. Fristrom, *SP357*, pp. 131-140 (June 1972).**

**Key words:** Chemical kinetics; combustion, gas phase; flame kinetics; flame mechanisms; flame suppression; inhibition; suppression.

A survey is given of the processes important in gas phase combustion with emphasis on chemical kinetics.

Gas phase combustion processes are important to the burning of polymers because the major exothermic reactions occur there. The combustion of many plastics can be roughly divided into a pyrolysis stage occurring at or close to the surface producing combustible gases and a gas phase oxidation stage in the surrounding atmosphere where the evolved gases are burned. Since the pyrolysis is usually endothermic, it is driven by the heat transferred from the gas phase flame by conduction and radiation.

Reaction schemes are outlined for some typical simple gas phase flames and these are related to the complex chemistry of the polymer combustion. A discussion is given of possible mechanisms for gas phase flame inhibition. Sources of information on chemical kinetics are listed and a bibliography is given of compilations of gas phase chemical kinetic rate parameters.

**Carbon formation in premixed flames, K. H. Homann, *SP357*, pp. 143-150 (June 1972).**

**Key words:** Acetylene-oxygen flame; benzene flames; bunsen flames; carbon formation; carbon limit; concentration profiles; cyanogen-oxygen flame; flame front curvature; hydrocarbon radicals; hydrogen diffusion; oxidation reactions; particle size; transport processes.

In this paper a survey is given on the processes leading to the formation of solid soot particles in premixed flames. Like most combustion products carbon formation is not exclusively determined by flame chemistry but is also dependent on transport processes. A local increase in the overall C/O ratio in the burning zone which is connected to the back diffusion of hydrogen and hydrogen atoms can reinforce carbon formation. This gives rise to the different types of carbon appearance in burner flames. It is shown that the C/O ratio at the site of carbon formation can be very different from that of the initial mixture.

For the formation of soot particles the presence of both highly unsaturated hydrocarbons and hydrocarbon radicals is necessary. The process of particle growth which cannot be described by equilibrium condensation theory shows two distinct phases: (1) A first phase of rapid growth which is due to the addition of higher unsaturated hydrocarbons to a particle surface with radical character. During this phase the number density of particles decreases while the individual particles retain their almost spherical shape. This is followed by (2) a phase of slow growth governed by the heterogeneous decomposition of a variety of unsaturated hydrocarbons on the particle surface which has lost most of its radical-like properties.

**Fluorocarbon combustion, fluorine supported combustion kinetics?, E. A. Fletcher, *SP357*, pp. 153-158 (June 1972).**

**Key words:** Chlorine; combustion; explosion limits; flame speed; fluorine; fluorocarbons; freons; ignition limits; kinetics.

Some interesting characteristics of the combustion behavior of freons and fluorocarbons are presented. The flame speeds and spontaneous ignition limits of chlorine burning in fluorine are easily described by simple models using well-characterized kinetics. The flame speeds of  $CF_3Cl-F_2$  and  $CF_3Br-F_2$  mixtures can be discussed in terms of simple thermal theories. The striking differences in the combustion behavior of homologous fluorocarbons are shown to depend on big differences in the rates at which the fuel molecules are initially attacked by the competitive combustion reactions, but the kinetics are not yet understood.

**Burning of polymers, C. P. Fenimore and F. J. Martin, *SP357*, pp. 159-168 (June 1972).**

**Key words:** Burning of polymers; flame retardants; flammability.

After a rod of solid polymer mounted vertically in a slowly rising stream of oxidant/inert gas mixture is ignited at the top end, the oxidant content of the mixture may be varied until that composition is found which will just support burning down the whole length of the sample. For many polymers this limiting volume-fraction of oxidant can be determined with a precision of about one percent and it serves as a convenient measure of flammability of the material.

Experiments show that the simplest model for such burning is one in which the oxidant does not react directly with the polymer, but is consumed in a nearby flame zone which heats and pyrolyzes the polymer to yield fuel gases. This model appears to be valid for some systems, but not for others.

Experiments may be carried out in which the compositions of the sample and the oxidizing atmosphere are varied in a systematic way. The measured flammabilities, together with a simple model of the burning process permit inferences about the manner in which composition variations affect the burning. The mode of inhibition by flame retardant additives may be inferred in this way.

For example an inhibitor which interferes directly with the gasification of the condensed phase should work independently of the flame reactions for the simple two-stage candle-like burning; it should still inhibit when the polymer is burned in  $N_2O$  rather than  $O_2$ . Such has been observed when chlorine has been substituted into polyethylene.

By contrast an inhibitor which poisons the flame reactions may be specific for reactions with oxygen and not work with another oxidant such as  $N_2O$ . Such is the case of  $Sb_2O_3$  added to slightly chlorinated polyethylene.

Effects of different inert gases, of initial temperature and of pressure have also been observed.

**Pyrolysis and combustion of cellulosic materials**, R. Alger, *SP357*, pp. 171-178 (June 1972).

**Key words:** Burning of polymers; cellulose; combustion of polymers; decomposition; fire spread; ignition.

Despite centuries of experience with burning cellulosic materials, men still do not agree on the interpretation of their observations. These divergencies of opinion generally involve mechanisms at the microscopic level where areas of ignorance still abound. This review deals with some of these opinions and the supporting experimental evidence pertinent to three chronologically related areas of fire research; namely, pyrolysis, ignition, and fire spread. Some of the ignition concepts and the models for fire spread are not limited to cellulose but should apply to a variety of solids.

**The surface pyrolysis boundary condition for the combustion of polymers**, R. F. McAlevy III, and W. S. Blazowski, *SP357*, pp. 185-192 (June 1972).

**Key words:** Combustion; flammability; kinetics; polymer burning; pyrolysis; rapid heating; surface pyrolysis; surface temperature measurement; thermal degradation.

The pivotal boundary conditions for polymer combustion involve the surface pyrolysis-vaporization characteristics. Generally, conditions at the burning surface (e.g., 500 °C or so) are so different from those encountered in classical bulk pyrolysis experiments that these data cannot be extrapolated reliably—data must be obtained at the conditions of interest. A critical review of experiments designed to produce such data, and the possible interpretations of these data are presented.

The authors have employed a combustion self-heating technique. In the experiment a planar diffusion flame is established between an axi-symmetric, "stagnation-point" flow of oxidant and the pyrolysis-product vapors emerging from the polymer surface lying below. The surface temperature, regression rate, and oxidant mass flow rate (the principal control variable) are measured. Recent results of this experiment are presented and discussed.

**SP358. 56th National Conference on Weights and Measures 1971**, F. C. Bell and H. F. Wollin, Report Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 358, 252 pages (Mar. 1972).

**Key words:** Administration, weights and measures; conference, weights and measures; laws, weights and measures; technical requirements, weights and measures; weights and measures.

This is a report of the proceedings of the 56th National Conference on Weights and Measures, held July 12-16, 1971, at the Shoreham Hotel, Washington, D.C., and attended by state, county, and city weights and measures officials and representatives of the Federal Government, business, industry, railroads, and associations.

**SP359. Metrology and standardization in less-developed countries: The role of a national capability for industrializing economies.** Proceedings of a seminar held at Airlie House, Warrenton, Va., February 1-4, 1971, H. L. Mason and H. S. Peiser, Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 359, 390 pages (Dec. 1971).

**Key words:** Africa; Asia; engineering standards; industrialization; Latin America; less-developed countries; measurement standards; NBS; quality control; U.S. AID.

The National Bureau of Standards held a 4-day Seminar in an effort to learn how its experience in metrology and standardization for the science and technology of U.S.A. might be used most effectively for less-developed countries. With financial support of the Agency for International Development, participants came from Argentina, Brazil, Ethiopia, Ghana, Guatemala, India, Israel, League of Arab States, New Zealand, Peru, and Vietnam; from several international agencies; and from industries, professional societies, and government in the U.S.A. The papers presented and the informal discussions were organized around the session titles:

#### Perspective

The Sociological, Economic, and Managerial Environment in Industrializing Countries

Making Scientific and Technological Measurement Meaningful

The Dissemination of Information

Promoting More Effective Use of Science and Technology

Additional Case Histories

Promoting Economic Strength and Commercial Equity

Guidance for NBS Technological Assistance Effort

It was concluded that industrializing economies would benefit from NBS activities in these fields, and specific suggestions were offered to that end. *These proceedings include the following papers (indented):*

**Objectives of the Seminar**, J. Bernstein, *SP359*, pp. 1-4 (Dec. 1971).

**Expectations from the Seminar**, L. M. Branscomb, *SP359*, pp. 5-8 (Dec. 1971).

**Keynote Address—The role of a national capability in metrology and standardization in industrializing economies**, J. D. Perkinson, *SP359*, pp. 9-13 (Dec. 1971).

**NBS programs to provide infrastructure services for science and technology in U.S.A.**, L. M. Kushner, *SP359*, pp. 15-23 (Dec. 1971).

**Overview—The anatomy of an industrializing economy**, G. Kalmanoff, *SP359*, pp. 31-36 (Dec. 1971).

**A case study from Latin America**, J. A. Sabato, *SP359*, pp. 37-41 (Dec. 1971).

**Labor saving versus capital saving industrial technology for the developing countries**, J. E. Stepanek, *SP359*, pp. 43-55 (Dec. 1971).

**The role of technology in politics and economics**, G. N. S. Maia, *SP359*, pp. 57-61 (Dec. 1971).

**Overview—The economic role of metrology capabilities**, E. U. Condon, *SP359*, pp. 71-78 (Dec. 1971).

**Needs for measurement controls in developing industrialization**, J. L. Hayes, *SP359*, pp. 79-84 (Dec. 1971).

**Problems in establishing accurate measurements in industrializing economies: A case-study of basic standards activities in the Israel NPL and some possible lessons to be learned**, H. Tabor and L. R. Farkas, *SP359*, pp. 85-90 (Dec. 1971).

**Instrument problems in a developing economy**, L. C. do Prado, *SP359*, pp. 91-94 (Dec. 1971).



Needs for standard reference materials for calibration and quality control, J. P. Cali, *SP359*, pp. 95-105 (Dec. 1971).

Overview—The role of Federal information activities, M. S. Day, *SP359*, pp. 115-125 (Dec. 1971).

Government responsibility for information for industry, A. Fontes, *SP359*, pp. 127-130 (Dec. 1971).

Publications: Documentation indexes, W. T. Knox, *SP359*, pp. 131-134 (Dec. 1971).

Extension productivity services via a developing country standards institute, P. M. Tam and N. C. Beck, *SP359*, pp. 135-141 (Dec. 1971).

Standardization in Africa: Problems and programs, Z. Fel-leke, *SP359*, pp. 143-149 (Dec. 1971).

Overview—The role of NBS capabilities, F. K. Willenbrock, *SP359*, pp. 159-162 (Dec. 1971).

Applying the computer, J. P. Nigro, *SP359*, pp. 163-165 (Dec. 1971).

Problems in industrial and technological research in Ghana, E. Lartey, *SP359*, pp. 167-171 (Dec. 1971).

Implementing metrology through operations analysis and systems engineering, S. E. Russek, *SP359*, pp. 173-175 (Dec. 1971).

Product development and market research, S. Marshak, *SP359*, pp. 177-180 (Dec. 1971).

The effect of local government policies on transfer of technology, G. E. Pratt, *SP359*, pp. 185-189 (Dec. 1971).

The sale of instrument manufacturing technology to small private industries in developing economies, P. K. Rohatgi, *SP359*, pp. 195-198 (Dec. 1971).

The Iranian Institute of Standards and Industrial Research, H. K. Work, *SP359*, pp. 199-200 (Dec. 1971).

Institutes for engineering education as a source of metrology, standardization and quality control in industrializing economies, P. K. Rohatgi, *SP359*, pp. 201-205 (Dec. 1971).

Design and development through metrology (abstract), P. Prakash, *SP359*, p. 206 (Dec. 1971).

Nondestructive testing, H. S. Peiser, *SP359*, pp. 207-208 (Dec. 1971).

Problems and attitudes in operating and maintaining a national standards laboratory in a small developing country, D. Pelli, *SP359*, pp. 209-211 (Dec. 1971).

Overview—The spread of standardization, F. L. LaQue, *SP359*, pp. 213-219 (Dec. 1971).

Overview—The role of standardization in industrializing economies, A. N. Ghosh, *SP359*, pp. 221-233 (Dec. 1971).

Weights and measures standards: laws, inspection, enforcement, M. Salama, *SP359*, pp. 235-238 (Dec. 1971).

The value of engineering standards in assisting industrialization in a less-developed country, R. B. Smith, *SP359*, pp. 239-242 (Dec. 1971).

The Colombia government faces the problem of quality control, H. F. Fernandez, *SP359*, pp. 243-247 (Dec. 1971).

Quality control and product certification, S. C. Le Roux, *SP359*, pp. 249-250 (Dec. 1971).

A systems approach to a conference synthesis, W. E. Cushen, *SP359*, pp. 257-264 (Dec. 1971).

Using national measurement standards, R. D. Huntoon, *SP359*, pp. 265-276 (Dec. 1971).

Preparing product specifications, N. A. Hall, *SP359*, pp. 277-280 (Dec. 1971).

Disseminating information, E. L. Brady, *SP359*, pp. 281-283 (Dec. 1971).

SP360. NBS 1971 Annual Report, T. M. Flynn, D. V. Baker, Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 360, 100 pages (June 1972).

Key words: Annual report, 1971.

This annual report is based largely on the testimony of Bureau management at the September 1971 Oversight Hearings. Significant events of the past year are included, as is a look forward where appropriate. The theme of the document, 70 years of service, is maintained throughout by means of photos from the historical files.

SP361. Volume 1. Performance concept in buildings. Invited papers. Proceedings of a symposium jointly sponsored by the International Union of Testing and Research Laboratories for Materials and Structures (RILEM), the American Society for Testing and Materials (ASTM), and the International Council for Building Research Studies and Documentation (CIB), Philadelphia, Pa., May 2-5, 1972, B. E. Foster, Editor, Nat. Bur. Stand. (U.S.), Spec. Publ. 361, Vol. 1, 819 pages (Feb. 1972).

Key words: Buildings; components; design procedures; experience in use; materials; performance evaluation; performance requirements; user requirements.

Volume 1 contains all of the invited papers accepted for the Joint RILEM-ASTM-CIB Symposium on the Performance Concept in Buildings. Opening addresses and reports of the rapporteurs will be included in Volume 2. The Symposium was held in Philadelphia, Pa. on May 2-5, 1972. The subject matter covered in the papers includes physiological, anthropometrical, psychological, sociological, and economic human requirements and methods of evaluation; physical requirements and methods of evaluation in mechanical, acoustical, thermal, dimensional stability, compatibility, fire properties, and geometry areas; operation and maintenance requirements and methods of evaluation in such areas as maintenance, repair, replacement, and versatility; techniques and problems in applying the performance concept to design; and experience gained in application of the performance concept in design, building, and building use. *These proceedings include the following papers (indented):*

Design specification—operational goals, parameters, synthesis, and performance criteria, J. F. Halldane, *SP361*, Vol. 1, pp. 1-12 (Feb. 1972).

Key words: Design evaluation; design specification; design synthesis; environmental systems; goal statements; parameter definition; performance criteria.

Evaluation, specification and monitoring in design has traditionally been based on the physical aspects of building environments. With a growing concern for human behavior there is a realization that the evaluation of environmental systems finally rests on whether the activities of people are satisfactorily supported by that system. Present methods of specification restrict the physical requirements in the in-

terests of behavior but fail to note the design goals that are intended to be addressed. Further, the categorization of parameters, both physical and non-physical, tend to be isolated into problem areas rather than groups that can be correlated. Performance is also narrowly interpreted in terms of physical entities alone.

A system is presented that coordinates environmental systems through a goal-parameter-synthesis-criterion specification which forms a base for design evaluation. The discussion includes the need for operational goals, a definition of non-physical parameters through an overt communication, a limiting stimulus system which links the organismic and environmental parameters, and criteria appropriate to the performance of operational goals. To illustrate the system certain lighting problems are studied from human behavior to light distribution. Rather than encouraging an attitude of regulatory compliance the system fosters alternative possibilities in design.

**Human requirements for buildings**, T. Cronberg, Å. Hallquist, R. Hansen, J. Nordan, and A. Saeterdal, *SP361*, Vol. 1, pp. 13-22 (Feb. 1972).

**Key words:** Human activities; performance criteria; physical environment; planning and design basis; user characteristics.

We build in order to establish certain required environmental conditions.

This set of conditions should be according to the users' requirements. This paper will discuss the users' activities and the users' characteristics as a basis for defining the users' requirements. Further we discuss a possible procedure for identifying the requirements and indicate the use through examples. The paper holds that it is necessary to take the variations in user's characteristics into consideration when defining the requirements. Further the paper tries to expand the use of users' activities to include all kinds of activities that may have consequences for the physical solution. The intention of what is put forward here is to initiate a further discussion of the continuation of this kind of work. It is not meant to give a solution to these problems.

**On structuring performance requirements for buildings**, T. Cronberg, A. Saeterdal, Å. Hallquist, and J. Nordan, *SP361*, Vol. 1, pp. 23-30 (Feb. 1972).

**Key words:** Organization of performance factors; performance requirements; required conditions; users' activities; users' characteristics.

This paper treats the problem of transforming users' requirements into relevant properties of a physical solution. From users' characteristics and activities we arrive at the required environmental conditions. Together with the data from the given conditions, this forms the basis for the performance requirements. These (data) must be structured in a way making it operative for design. By classifying the requirements according to their basic functions we are able to get from this point to a set of properties relevant for a chosen type of physical system.

**Performance requirements of the thermal environment for human occupancy**, R. G. Nevins and P. E. McNall, Jr., *SP361*, Vol. 1, pp. 31-42 (Feb. 1972).

**Key words:** Air motion; air temperature; comfort; mean radiant temperature; performance; relative humidity; thermal environment; thermal neutrality.

Recent physiological and psychological research is analysed from an engineering point of view to determine the

ranges of the variables which provide satisfaction with the thermal environment. The preferred values of the thermal variables, dry bulb temperature, mean radiant temperature, water vapor pressure in the air and air velocity, are presented for various levels of activity and clothing. Permissible steady-state deviations are defined for practical satisfactory environmental control. The effect of variations with time is discussed and recommendations are given for limiting criteria. The environmental variations associated with different human activities and clothing ensembles are analysed.

The necessary shift in dry-bulb air temperature to maintain subjective comfort in response to variations in the other thermal parameters is presented as the suggested functional requirement and as a means for assessing the quality of existing or proposed environments. Simulation of the total building system is suggested including Man, the Building, Climate and the Environmental Control System. A man-analogue is described for use with design simulation models or for performance ratings with on-site measurements.

**Performance requirements of buildings and the whole problem**, W. M. Peña and J. W. Focke, *SP361*, Vol. 1, pp. 43-55 (Feb. 1972).

**Key words:** Analytical procedures; architectural programming; buildings; performance requirements; problem seeking; statement of the whole problem; user needs.

Because so many groups of people (the client owner group, the client user group, and governmental agencies) participate in establishing performance requirements for an architectural project, the approach must be rational enough to withstand public scrutiny and analytical enough for the data to be classified and interrelated for greater mutual understanding.

Programming is a process leading to the statement of an architectural problem and the performance requirements to be met in offering a solution. Architectural programming is problem seeking, resulting in those qualitative and quantitative statements that describe the whole problem in terms of function, form, economy and time. The performance requirements deal with what is to be achieved without regard to the physical response.

The search for performance requirements is evident in each of the five steps of the programming process which follow:

1. Establish Goals (Qualitative)
2. Collect, Organize and Analyze Facts (Quantitative)
3. Uncover and Test Programmatic Concepts (Qualitative)
4. Determine Needs (Quantitative)
5. State the Problem (Qualitative)

The steps and considerations form an analytical framework for classifying and processing data (coming from sources) into information. This framework is also useful in avoiding information clog and as a format for dialogue among the many participants.

A typical problem can involve the rote application of a hardware system without concern for the user. However, if the approach emphasizes the performance requirements of the user, then we have defined a unique problem. A hardware system may then be a part of the solution but it will be applied in the context of the whole problem.

**Performance requirements of housing in response to the life cycle: a behavioral approach**, L. A. Pastalan, *SP361*, Vol. 1, pp. 57-62 (Feb. 1972).



**Key words:** Age and perception; complexity; home range; life cycle; life space; loss continuum; macro space; mastery; micro space; redundant cuing; sensory acuity; sensory deterioration; spatial sets; user needs.

This paper concerns the development of a conceptual model dealing with performance requirements of housing in response to the changing physiological and psycho-social needs over the life cycle of the user.

The model relates the range of user needs to the human development continuum beginning with infancy and its extension to old age (100 years plus). Attention is focused on physiological and behavioral change from development in infancy and young adulthood to deterioration in old age. Changes over time in sensory acuity, energy levels, health status and activities of daily living are linked to three basic propositions regarding residential environments and user requirements: 1) The stimulus function must respond to differential sensory changes over the life cycle; 2) The orientation function of residential spaces must have high predictive value for young children and old people as well as young and middle-aged adults in order to elicit behavior appropriate to the setting; and 3) Spaces must be organized in such ways as to assure the expression of autonomy or jurisdictional control over personal space of each user while at the same time providing opportunities for social interaction with significant others.

**Performance of systems of constructed facilities, A. C. Lemer and F. Moavenzadeh, *SP361*, Vol. 1, pp. 63-71 (Feb. 1972).**

**Key words:** Maintainability; measures of effectiveness; multidimensional decisions; reliability; subjective evaluation.

The performance of a constructed facility must be evaluated in terms of the facility's role within the larger social-economic-political system of which it is part. It is suggested that performance may be measured in terms of three principal parameters: serviceability, reliability, and maintainability. Serviceability is the degree to which the facility provides satisfactory service to the user, here understood to include a broad range of the recipients of benefits of the facility. Reliability is the probability that service will be adequate throughout the design service life of the facility. Maintainability is a measure of the degree to which continuing effort is required during the service life to keep serviceability at an acceptable level. This approach emphasises the user as a basis for evaluation, and the need to consider the entire service lifetime of a facility in decision. The implementation of procedures to permit usage of these parameters in decision-making requires application of techniques from psychology and economics, and from probability theory.

**The relationship of the performance concept to the planning process—developing performance requirements for community mental health centers, D. B. Hattis, *SP361*, Vol. 1, pp. 73-82 (Feb. 1972).**

**Key words:** Building procurement; building systems; hospital planning; office building; performance.

The performance concept is best explained as the description of a system in terms of its output rather than its parts. When this concept is applied in the procurement process of any system the formal instrument used to effect the procurement is a performance specification.

Several advantages of performance specifications over prescriptive specifications have been suggested, particularly in the areas of economy and technological innovation.

When applied to building, performance specifications can be used at various scales of elements or systems, thus producing a "hierarchy of performance." It has been found that when used at a particular scale, the need to define the scope of the system of a performance specification requires the prescription of elements at the next higher scales.

There are several criteria for determining the scope of a system to be used on any particular project, but in general it is easier for "clear" building types than for "ambiguous" ones.

In attempting to define the scope of a system for "ambiguous buildings," one often finds oneself substituting the question "What is a house?" for the question "How should a house perform?" The former question leads to concern for earlier decisions in the planning process.

**Institutional performance and building performance: some implications of the Judicial Facilities Study, B. Handler, *SP361*, Vol. 1, pp. 83-91 (Feb. 1972).**

**Key words:** Activities; communication; courthouse; human performance; institutional performance; judicial system; mutual adaptation; objectives; operations; physical determinism; physical environment.

The performance of the institution or organizations which buildings serve has not been regarded as within the province of architectural analysis. Failure to evaluate institutional requirements can result in buildings which hamper rather than help the performance of institutions. A critical examination of the objectives and operations of the judicial system was a major theme of the Judicial Facilities Study, designed to develop standards and guidelines for courthouse design in the United States. How these facility standards were derived from a detailed examination of the judicial system is explained in terms of: the ways in which judicial system requirements and personal human requirements were handled; the present and future purposes and human needs the system and its facilities seek to fulfill; the manner in which the operations of each court function and specialized proceeding were examined; the ways in which activities, interpersonal relations, communication patterns, environmental and spatial characteristics were analyzed. Certain conceptual and theoretical considerations implicit in the approach to the study are discussed. The assumptions of conventional architectural analysis are stated, and the physical determinism inherent in them criticized. An alternative hypothesis is advanced, namely, that the effect of the physical environment on human performance varies with institutional performance. Buildings and the operations of the institutions they house are seen as interdependent, mutually adapting to each other as the people involved attempt to achieve correspondence between the two. The ideal of perfect consonance is viewed as able to be approached only if the designer has a thorough understanding of the institution both as it is and as it ought to be.

**The complementary use of research and negotiations with users in the development of performance standards, T. Mann and R. Bender, *SP361*, Vol. 1, pp. 93-100 (Feb. 1972).**

**Key words:** Arguments; decision-making; IBIS (Issue Based Information System); negotiations; research, structured planning discourse; user needs, aspirations, values.

Two assumptions underlying much of the current discussion about industrialized building systems for housing are: (1) research should investigate the needs of users of housing, and (2) the resulting findings can be cast into explicit performance standards or specifications to permit industry to

develop and mass produce housing systems conforming to these standards and to the needs of users.

These assumptions are questioned. If user requirements research is to produce useful results, it must focus upon users in actual decision-making situations and be complemented with procedures of negotiation, conflict-detection, argumentation, debate, bargaining and conflict-settling.

An approach is discussed which puts research into the implementation phase of actual projects as a part of the planning discourse and decision-making process.

**Application of unobtrusive observation techniques in building performance appraisal**, W. F. E. Preiser, *SP361, Vol. 1*, pp. 101-109 (Feb. 1972).

**Key words:** Behavioral cost; building performance; cultural context; unobtrusive observation; user behavior; user feedback.

The performance of buildings is commonly measured in economic terms such as return on investment, or in otherwise readily quantifiable terms, such as amount of time required for maintenance, heat transfer, acoustic properties, or durability of materials. "Behavioral cost," which might be defined as dysfunctional aspects in the human organism caused by elements in the social and the designed environment, traditionally has escaped rigorous measurement and quantification. It became evident only through indirect indices such as statistics on pathologies, absenteeism, job turnover, etc. It is suggested that in addition to the commonly used performance measures, building performance be based on normative user behavior that is explicitly stated in building program specifications. Several approaches to this problem area are outlined.

A performance evaluation study in a public plaza using observational techniques is reported. The findings indicate that a strong relationship exists between informal stationary activity and space defining elements in the plaza, such as benches and columns. Certain conclusions for the programming of a plaza are drawn.

**Verbalized user response and the building performance concept: a case study in university residence hall evaluation**, W. F. E. Preiser, *SP361, Vol. 1*, pp. 111-119 (Feb. 1972).

**Key words:** Attitude scale; building performance; comparative user response; user behavior; user satisfaction; verbalized response.

Building performance appraisal focused upon user behavior is a recognized need. Theoretical frameworks exist for the analysis, programming, and design of buildings with human behavior as the basic unit of analysis, particularly with reference to normative states of equilibrium within a given cultural and environmental context. These states may be expressed in terms of user satisfaction through verbalization. Based upon Thurstone's scale of equal-appearing intervals, an evaluative tool for the qualitative assessment of building performance has been developed. The method attempts to measure the subjective importance and acceptance of features of the built environment by the users. The data thus derived may complement traditional "hardware" criteria in the appraisal of buildings. The evaluation procedure, consisting of six steps, was applied to students living in residence halls at Virginia Polytechnic Institute and State University.

1. Construction of Attitude Statements.
2. Selection of Statements.
3. Scaling of Attitude Statements.
4. Statistical Evaluation.
5. Selection of "Best" Scoring Statements.

**6. Validation Procedure and Construction of Comparative Response Profiles of 3 Residence Halls.**

Some conclusions resulting from the building evaluation are outlined for consideration in future programming of residence halls.

**Identification of performance criteria using multidimensional scaling of user evaluations**, H. G. Blasdel, *SP361, Vol. 1*, pp. 121-129 (Feb. 1972).

**Key words:** Color schemes; field studies; glare; illuminance; matrix analysis; multidimensional scaling; performance criteria; preference scaling; scaling; user evaluations; visual environment.

The relative significance, accuracy and completeness of performance criteria for environmental control systems in buildings require testing through user evaluations in addition to customary laboratory research. Because of the inherent variability in human judgment, and the difficulty of interpreting direct quality estimations, such evaluations have not been widely used. Multidimensional scaling allows the reduction of comparative evaluations into a quantitative system of perceived environmental attributes. A questionnaire was used in evaluation of luminous environments as an example of the technique. Results provide for identification of perceived attributes and the scaling of the observed environments with respect to those subjective parameters so that physical measures may be related to human responses.

These methods differentially weight the salience of each attribute for each individual's judgment matrix, allowing access to data on individual differences that can assess the need for variety in a building system. The attribute structures may be applied to setting quality criteria across a wide range of environmental variables so that cost-benefit analysis may be done against overall performance rather than separate criteria.

**Performance: the new language of design**, D. J. Parsons, *SP361, Vol. 1*, pp. 131-139 (Feb. 1972).

**Key words:** Cost; design; industrialization; performance; user needs; value system.

With the scattered development of tools for user needs analysis, the measurement and specification of performance, product analysis, and building evaluation, there is a growing need for unification of these concepts into a single framework. A definition of the performance concept is presented which mediates between the measurement of benefit and the costs of design solutions. With performance as a mediating concept, we are able to formulate user needs as the correlation between performance and benefit, and to analyze products in terms of the relationship between their cost and their performance. The Performance/Benefit correlation (user need) is a user characteristic *independent* of product Cost; while the Cost/Performance relationship is a product characteristic *independent* of Benefit to the user. This paper clarifies the relationship between this definition of the performance concept and various forms of analysis, design, and evaluation common to the design of buildings. It further explores possible shifts in the practice of design as skills become more specialized in the building industry.

**Consideration of externalities to the basic performance/cost evaluation of buildings in the design process**, G. S. Birrell, *SP361, Vol. 1*, pp. 141-148 (Feb. 1972).

**Key words:** Building; competitive market; construction; cost; evaluation; materials; performance; price; user; value.



Starting from (1) an adequate analysis of buildings into subsystems and their functional elements; (2) the statement of required technological performance for each element of a proposed building; and (3) the budget cost for each element of a proposed building, the question arises—what else should the designer include in his evaluation of each building element to maximize overall User Satisfaction?

These externalities to the basic technological performance and cost of each element are described and discussed and their relationship to each other exposed on a Value Axis. They comprise a range of factors from Hypothetical Minimum Cost to User Values. They are interrelated and influenced by the Project Roles which are responsible for each section of the Value Axis on each Project. Such externalities play an important part in the integration of the elements to create a desirable overall project and the designer should direct his attention to them to achieve optimum overall balance between Performance and Cost.

The conclusion reached is that while the above ratio of technological performance to cost of each element is a desirable starting point for building evaluation, the externalities on the Value Axis also play a considerable part in selecting the building materials which can provide maximum building User Satisfaction.

**Architectural economics related to comfort, productivity and glass,** J. T. Malarky, *SP361, Vol. 1*, pp. 149-159 (Feb. 1972).

**Key words:** Building economics; capital costs; human comfort; human performance; insulated glass; operating costs; people costs; single glass.

For many years, the most sophisticated and objective professionals have believed that thermal and visual “environmental factors” can exert a profound influence on the physical comfort and productivity of building occupants. Some experienced owners, such as the General Services Administration, believe that 90 percent of the owners’ total cost in an office building can be charged properly against people and only about 10 percent against land, building and debt service. Experienced tenants regularly pay more money for carefully controlled and selected environments.

Glass “environmental factors” such as glass surface temperature, influence productivity and can be evaluated in a practical way. For exploratory use and for professional evaluation and criticism, an empirical people-productivity/glass-performance evaluation system is proposed. This evaluation system illustrates a practical relationship between glass “environmental factors,” comfort and productivity. A comfort-productivity relationship equation is developed. A practical example illustrates the effect architectural glass could have on productivity and profits.

**The notion of performance in building: building requirements,** G. Blachère, *SP361, Vol. 1*, pp. 161-164 (Feb. 1972).

**Key words:** Assembly; compatibility of components; physical properties of a building, of a product; users’ requirements.

A building is built for a given purpose, i.e., to meet the requirements of the man for whom the building is built, the user’s requirements. These are related to the whole building and can be expressed in terms related to man by numerical figures for the best known requirements such as physiological and economic ones, and by words in other cases, i.e., for psychological or sociological needs, roughly speaking.

To meet the users’ requirements, a building has to present a set of physical (including chemical, geometrical, and mechanical) properties. Various sets of physical properties may be suitable to meet the same set of requirements.

Generally speaking a building is built of elements, and elements are made of products (raw materials, semifinished products, sections, components).

It is possible to relate the properties of a built element to the properties of the constituent products, by considering the various physical characteristics and also the compatibility of adjacent parts.

Some details will be given on the users’ physiological, psycho-sociological and economic requirements at the level of the whole building; on absolute needs and relative requirements; on the variation of requirements in space and time.

**What are the natures of performance and evaluation for the three levels: building, components, materials,** G. Blachère, *SP361, Vol. 1*, pp. 165-170 (Feb. 1972).

**Key words:** Agrément; building components; durability; materials; performance; tests.

For a whole building what is required is the satisfaction of the users’ requirements. For example for a dwelling the requirements are temperature, noise level, illumination level, air purity level, convenience of internal space, convenient relationship between the various rooms and an adequate view from the inside, etc.

The means of evaluation are the sciences which relate the physical properties of the building to the effect on the inhabitants, or reference to a long and satisfactory use of some techniques or direct proof by the real occupation of the building by users and the observations of the latter.

What is needed for components is that they possess the physical properties which enable the built elements to play their correct part in the building as a whole.

These properties are expressed in scientific terms, i.e., by reference to physical characteristics measured by any methods, in terms of technological indexes based on long experience or on tradition, or in terms of physical requirements. There is also the important problem of durability (cf. the paper on Agrément).

As for raw materials, it is not possible to have requirements of any sort by performance or otherwise, because there is no defined link between materials and a building. We can only judge a material plus its shape, i.e., roughly speaking, a component.

**Techniques for developing performance specifications for buildings,** M. Brill, *SP361, Vol. 1*, pp. 171-180 (Feb. 1972).

**Key words:** Environmental characteristics; performance; performance specifications.

A tested technique is offered, which can serve as a generating model for performance specifications for any building type. The technique recognizes the primacy of the user’s needs as the generator of information, while acknowledging that manufacturer’s information requirements must be formatted in different terms. A matrix is used as a display device to show the set of all possible environmental characteristics for all possible subsystems.

The environmental characteristic headings are: Conditioned air, Illumination, Acoustics, Stability, Durability, Reliability, Safety, Activity support, Maintainability, Esthetics, Waste management, Potable water, Food handling, Communication, Accessibility.

The Building subsystems whose performances must satisfy these requirements are: Structure, HVAC, Finished floor, Finished ceiling, Luminaires, Space dividers, Exterior walls, Plumbing Utilities, Sanitary fixtures, Food services, Cleaning systems, Energy source, Energy systems, Transportation systems, Roofs, Windows, Doors, Security

systems, Sealant systems, Communication systems, Materials handling, Waste removal.

Each intercept is examined for interaction between demand (the user's needs) and supply (the capability of the subsystem to respond to, or alter the demand). Where an intercept is seen as interactive, three kinds of information are generated—a *Requirement* which is a prose statement of the specific need; *Criteria*, some measure of the acceptable range of solution; and *Test Method*, the mechanism whereby surety of performance is guaranteed. A method of correlating Requirements, Criteria, and Test Methods into performance specifications by subsystem is described.

This technique attempts to deal with physiological requirements only and some discussion is presented for its applicability to psychological and sociological requirements.

**A consistent basis for functional and ultimate criteria**, R. N. Wright and A. H.-S. Ang, *SP361, Vol. 1*, pp. 181-190 (Feb. 1972).

**Key words:** Building criteria; design; optimization; reliability; safety; serviceability; structures.

Objectives in the process of building include minimization of cost as well as performance in meeting functional requirements and safety with respect to property loss or personal injury. The performance concept contributes to these objectives by expressing performance requirements in a manner allowing fair competition among available solution schemes. This paper discusses the formulation of functional and ultimate criteria for structural performance using rational consideration of uncertainties in the information available for decision making.

Functional requirements define limit states of serviceability which are independent of solution scheme. Requirements for safety, however, relate to ultimate limit states which differ in mechanisms and consequences for different structural schemes. This paper shows that performance requirements for safety can be expressed in a scheme-independent manner by accounting for the scheme-dependence of ultimate limit states with reliability-based criteria.

Total performance is described by the expected loss which includes expected initial costs and probable costs of occurrence of functional and ultimate limit states. This formulation guides the expression of performance requirements in ultimate limit states as scheme-independent prescriptions of required reliability. Both statistically defined and statistically undefined uncertainties are accounted for. The fail-safe concept provides very high reliability against catastrophic ultimate limit states.

**Performance concept and the system approach—some comments**, I. Karlén, *SP361, Vol. 1*, pp. 191-200 (Feb. 1972).

**Key words:** Building; design process; ER-system; performance; performance concept; quality description; system approach.

This paper will comment on two main approaches for use of the performance concept: behaviour in use and output of a process. The system approach, applying inter alia the performance concept, can be used in different stages of the building process, particularly for description of the wanted result, the final system. The author tries to give examples of applications on different product levels. The ER Quality description system is one example. The author comments on the help given by classification in the applications and the relations between classification categories, levels and classification.

**The performance concept in building: the working application of the systems approach to building**, R. G. Robbie, *SP361, Vol. 1*, pp. 201-206 (Feb. 1972).

**Key words:** Buildings; design process; performance; performance concept; performance-judgement approach; proposed international generic building classifications; proposed international subsystem classification models; systems approach; user needs.

The paper reviews the meaning of the systems approach to building in its practical context. Attention is drawn to the local factor in building when consideration is given to performance requirements. A characteristic which separates theory from accomplished practice in building. It is suggested that the local factor in building could make the notation of the pure performance approach to building something of a hoax, or at least common and current misconception in the industry. The realities of building performance assessment on major systems programmes are noted and a suggestion is made that the concept of the (pure) Performance Approach or Concept of Building should be discarded. It is recommended that the Performance Judgement Approach or Concept be adopted as a more accurate representation of the daily realities of performance-based building practice.

The paper proposes the establishment of an international Generic Building Classification for the bulk of common building uses. It reviews the apparent divergent meaning of performance specifications as they appear to be finding application in Europe and North America. A proposal is made for the establishment of international sub-system classification models and two examples are given for schools and housing.

The paper concludes with an appeal for a major increase in user requirements research and the development of science-based skill in the building industry. It appeals also for a major rationalization of all skills in the industry in the expectation that with building code rationalization the building industry would then have the comprehensive resources necessary to make the performance concept in building a reality.

**The relationship between the performance concept and the systems concept**, J. Vilett, *SP361, Vol. 1*, pp. 207-212 (Feb. 1972).

**Key words:** Building industry; building production process; building systems; innovation; performance approach; semantics; systems approach.

There is considerable confusion in current architectural, engineering and construction literature concerning the distinction and relationship between the performance and systems concepts. It would be useful to maintain a clear theoretical separation of these ideas. Although there is value in their simultaneous application to many types of project, each also has the capability for independent application to certain aspects of the building process. The rationale for this proposition is based on a comparative analysis of the two concepts in terms of definitions, objectives, origins, scope of applicability, and advantages and disadvantages.

**Computer based code systems and the performance concept**, J. P. Eberhard, *SP361, Vol. 1*, pp. 213-218 (Feb. 1972).

**Key words:** Building codes; building systems; computer systems; performance standards; simulation of building requirements; systems design.

Building codes are part of a building code system which is intended to provide an organized process by which such codes are: communicated, updated, enforced, administrated



and evaluated. Historically this code system has been manually operated by the use of printed documents. There is some evidence to indicate that it would be economically and technically possible to convert most of this system to one which was computer based. A computer based code system could be self-improving, resource conserving, provide an information based to the design process, raise the level of sophistication of evaluation methods, and make the code requirements more nearly responsive to the performance requirements of building users.

**Performance analysis,** Tenho Sneek, J. Saarimaa, and Timo Sneek, *SP361, Vol. 1*, pp. 219-226 (Feb 1972).

**Key words:** Application of performance concept; building levels; external factors; internal factors; performance analysis; performance evaluation; stages of building.

A performance analysis technique for building elements, products and materials is described. In order to be able to evaluate the total performance of an object all influencing factors must be known. The technique is based upon the listing of the external factors affecting the object. The internal factors of the object have to withstand the effects of the external factors. By juxtaposition of the external and internal factors, requirements concerning the desired properties can be written. The analysis can be made by the aid of check lists for external and internal factors.

**Building performance appraisal,** T. A. Markus, *SP361, Vol. 1*, pp. 227-235 (Feb. 1972).

**Key words:** Appraisal; building performance; constraints; environmental system; evaluation; resources.

This paper outlines a model of an interactive system with five main components:

1. the goals and objectives of an organization;
2. the activity and behaviour appropriate to the achievement of these objectives;
3. the environment suitable for the activity;
4. the hardware required for the creation of a suitable environment; and
5. the resources required as inputs into the system and the values achieved as outputs.

It sets out the main stages in appraisal—modeling, measurement and evaluation, and then discusses the role of performance criteria under three categories: the “ideal,” norms and constraints. The paper concludes with a brief reference to a published appraisal of a school and some of the findings resulting from it.

**A systems approach for the evaluation of performance of buildings in design process,** S. G. Haider and N. Khachaturian, *SP361, Vol. 1*, pp. 237-248 (Feb. 1972).

**Key words:** Building design; design process; evaluation; performance; systems approach; user requirements; value system.

Buildings are man-made physical systems which are essential, in one way or another, for almost all activities in the society. The worth of a building is some combined measure of its performance in the functional, technological, economic, perceptual-aesthetic and sociological contexts. However, most of the work done in the evaluation of performance of buildings has been directed to specialised aspects within isolated contexts and is often limited to particular types of buildings. There is a need for considering the evaluation of overall performance of a building within the design process framework of a building as a system. This

paper is intended to be a step towards the fulfillment of this need.

In the design process, the concept of value system that forms the basis of performance specifications and criteria; synthesis of building scheme which specifies the form, materials and construction methods; and operations on information are briefly discussed. The value system is systematically analysed into criteria and constituent measures which in turn are shown to be functions of design parameters and performance variables of building scheme. The evaluation process starts with the performance ratings at the level of constituent measures and successively integrates them into a single measure of the overall worth of the building design.

**An innovative approach for building system analysis and design,** M. J. Macalik, *SP361, Vol. 1*, pp. 249-253 (Feb. 1972).

**Key words:** Building system analysis; design; innovation; mathematical model; predictive technique.

The intent of this paper is to introduce a new computer program formulated to aid in the evaluation of performance of building systems and components. The new program is designed to define, within a range of possibilities, the scope of future innovation in building systems and components necessary to improve their performance for the user and their profitability to the manufacturer.

**A general overview of operation BREAKTHROUGH,** E. V. Leyendecker, *SP361, Vol. 1*, pp. 255-260 (Feb. 1972).

**Key words:** Department of Housing and Urban Development; housing; industrialized housing; innovative housing; National Academies of Sciences and Engineering; National Bureau of Standards; Operation BREAKTHROUGH; performance; performance criteria.

Operation BREAKTHROUGH was initiated with the overall objective of increasing housing production by breaking through the barriers which constrain the use of innovative materials and systems in producing housing. Twenty-two housing systems were selected by the Department of Housing and Urban Development (HUD) to participate in the program by erecting housing on selected prototype sites. The Building Research Division of the National Bureau of Standards (NBS) was selected to write performance based criteria and evaluate the housing for HUD. A technical panel formed by the National Academies of Sciences and Engineering is providing HUD with independent advice on the results of the NBS evaluations.

**Philosophy and scope of structural performance criteria,** F. Y. Yokel and N. F. Somes, *SP361, Vol. 1*, pp. 261-266 (Feb. 1972).

**Key words:** Deflection; load capacity; performance criteria; performance evaluation; stiffness; strength; structural engineering; structures; user requirements; vibration.

In the program entitled “Operation BREAKTHROUGH,” the U.S. Department of Housing and Urban Development is supporting and guiding the development of industrial housing systems and encouraging innovation in housing technology. Evaluation criteria that were developed by the Building Research Division of the National Bureau of Standards’ Institute of Applied Technology will be applied to all “Operation BREAKTHROUGH” housing systems. This paper presents the philosophy for the development of Structural Performance Criteria, which are derived from the user requirements of safety, activity support, low maintenance

cost, absence of stress and anxiety and visual acceptability. One example is quoted to illustrate the form of these criteria, which comprise three groups: strength, stiffness and rigidity, and resistance to local damage.

**Philosophy for physical simulation using performance criteria**, N. F. Somes and F. Y. Yokel, *SP361, Vol. 1*, pp. 267-274 (Feb. 1972).

**Key words:** Accelerated aging; building systems; extreme loads; performance criteria; performance evaluation; service loads; stiffness; strength; testing; variability.

Physical simulation may be defined as a testing procedure designed to closely simulate the actual structure in order to determine the response of the prototype structure to the loads it is likely to receive during its service life. Criteria for physical simulation include the selection of critical assembly, the consideration of critical load conditions, the allowance, the allowance for the effects of the service life environment and taking account of variability in structural elements and subsystems. The paper discusses each of these criteria in detail, and presents a philosophy.

**Field testing of conventional buildings for static and dynamic deflections**, G. C. Hsi, H. S. Lew, F. Y. Yokel, and N. F. Somes, *SP361, Vol. 1*, pp. 275-288 (Feb. 1972).

**Key words:** Building; design criteria; drift; field test; floor vibration; wood frame.

In order to evaluate innovative materials and systems it is necessary to develop performance criteria for aspects of structural behavior which hitherto have not been considered for traditional materials and solutions. It is reasonable to set levels of performance required by these new criteria so as to achieve a performance which has been acceptable to society over a long period of time. Unfortunately, there is a lack of data on the performance of traditional buildings. This paper describes recent field testing of several conventional buildings in order to confirm the suitability of performance criteria established for static and dynamic deflections within the "Operation BREAKTHROUGH" program.

**Performance of components: a procedure for the preparation of specifications for building components**, H. W. Harrison, *SP361, Vol. 1*, pp. 289-296 (Feb. 1972).

**Key words:** Building components design; building procedures; contracting procedures; performance specifications; properties of building materials; standardization.

The United Kingdom Building Research Station has been assisting a number of public bodies—central government departments, or consortia of local authorities—in the preparation of performance specifications, and monitoring their use in the purchase of components for educational, housing and other building programmes. The procedure used is described. Reference is made to the problems involved in obtaining alternative proposals from manufacturers and in assessing their suitability, also to the use of the CIB master list of properties.

**User requirements and performance design**, J. King, *SP361, Vol. 1*, pp. 297-301 (Feb. 1972).

**Key words:** ABS (Academic Building Systems); EFL (Educational Facilities Laboratories, Inc.); environmental criteria; evaluate; performance criteria; performance design; RAS (Recherches en Amenagements Scolaires); SCSD (School Construction System Development); SEF (Study of Educational Facilities); SSP (Schoolhouse Systems Program); URBS (University Residential Building System); user requirements.

To establish performance goals for buildings based on extensive user requirement studies has been the basic underlying goal behind the building systems which have been developed for educational buildings in North America. Evaluating the quality of buildings has generally been a subjective question. Establishing performance criteria begins to tie quality to measurable objectives rather than more ephemeral issues. Finding those performance objectives which can be described, which are relevant to the building, which are relevant to education, and which protect the economic interests of the owning institution is neither simple nor direct. Conflicts between immediate economic advantage and long range flexibility, between comfort and economy, between low first cost and long-range operational economy make for difficult decision making.

Weighing the comparative importance of the conflicting interests of the user-client (student/teacher/dormitory resident) and the owner-client (school system/college/university) is the most subtle area of decision making and the toughest. The evaluation of whether the resulting buildings meet the performance criteria is a comparatively simple matter. Reexamining whether the performance criteria adopted was appropriate and consistent with the direction the institution has taken since the building has been built, occupied and used is a more significant and of course a more difficult question to get at.

**Paths to performance—some recent projects employing the performance concept**, W. Meyer, R. Bender, and C. Arnold, *SP361, Vol. 1*, pp. 303-315 (Feb. 1972).

**Key words:** ABS; building systems; college buildings; dormitories; HVC; laboratories; lighting/ceiling; performance specifications; procurement process; SCSD; structure; subsystem; URBS.

Two building research, and development programs, organized and directed by our firm (BSD), have utilized the performance concept, each with a different approach and end result. Both projects were based on earlier experience coordinating the School Construction Systems Development (SCSD) program.

Based on an analysis of user requirements, performance specifications and/or requirements were developed on the URBS (University Residential Building System) program for University of California student housing, and on the ABS (Academic Building Systems) program for Indiana University and University of California academic buildings.

The URBS project involved performance specifications to guide the development by manufacturers of five new subsystems for student housing. Specifications for the subsystems were written to accommodate cooperation between bidders and to assure an integrated design proposal. Product development to meet the URBS performance specifications was based upon a large, guaranteed market. The ABS program on the other hand, could not guarantee a future market and therefore assumed the selection of existing, already developed, products for its five subsystems.

Based on the experience gained from the URBS and ABS projects, the paper calls for the encouragement of public agencies to collect and develop, as necessary:

- methods expressing man's environmental needs in performance terms;
- scales for displaying various levels of performance;
- methods for relating levels of performance to various activities or spaces as they occur in buildings; and
- models for using performance-oriented requirements in building and building systems procurement processes.



The "Recherches en Aménagements Scolaires" (R.A.S.) project— a case study—strategy implemented for the development of a building system for educational facilities through the Performance Concept, M. Bezman, *SP361, Vol. 1*, pp. 317-330 (Feb. 1972).

Key words: Bid evaluation; building systems; criteria and tests; educational facilities; life cost; performance specifications; prototypes; S.C.S.D., R.A.S.; strategy; systems approach; technology and feasibility; user needs.

The R.A.S. Project (Research in School Facilities), was conducted by the author for the Montreal Catholic School Commission. Both the recognition of a basic problem common to all school districts, and the acceptance of a problem solving direction experimented with in California through the S.C.S.D. Project, are at the origin of the R.A.S. Project. The problem is the inadequacy of traditionally accepted methods to provide educators with appropriate and adaptable facilities within limited financial boundaries and the direction is the adoption of the "Systems Approach" for viewing and solving the problem, and the "Performance Concept" as a means for achieving the objectives subsequently defined.

The Performance Concept approach was instrumental in harnessing Canada's industrial resources and potential for the development of a building system (presently under implementation) integrating the following sub-systems:

1. Structural
2. Heating-Ventilation-Cooling
3. Ceiling-Lighting
4. Internal Space Subdivision
5. Electric-Electronic Distribution

The strategy enforced and the means implemented through the various stages of the project, as well as the subsequent results are discussed throughout.

The paper covers:

- the project's specific context,
- the main surveys conducted to establish a basis for Performance Specifications, from user requirements to evaluation of resources,
- the major Performance Requirements developed to identify the problems for which a solution was sought,
- the Performance Criteria defined to qualify and quantify the required levels of performance,
- the evaluative methods implemented during the pre-bid, bidding and development phases of the project (scientific measurement, empirical evaluation and economic evaluation) to test and evaluate the building systems "as a whole" and at the level of their individual sub-systems.

The development of performance criteria for university facilities, R. F. Hallenbeck, *SP361, Vol. 1*, pp. 331-337 (Feb. 1972).

Key words: Acoustical environment; administrative procedures; communication; environmental criteria; functional criteria; interior finishes criteria; luminous environment; measurement; outdoor lighting criteria; performance criteria; process description; university facilities.

Since its inception in 1962, the State University Construction Fund has been responsible for the planning, design and construction of campus facilities for the State University of New York. It is estimated that as of September 1971, the Fund has completed, or placed under design or construction, facilities costing 2.31 billion dollars. In concert with this large-scale effort, the Fund has undertaken the development of performance criteria for its physical facilities in two

groupings— Environmental Performance Criteria and Functional Performance Criteria. It is contemplated that criteria in these two areas will be synthesized into a third area of criteria for Construction System Performance upon completion of research in progress. Difficulties in generating industry wide acceptance of measurable performance criteria has lead to the exploration and development of a variety of means of communicating Fund requirements to the design professionals who prepare plans and specifications for university facilities. These interim approaches to communication of performance requirements include: State-of-the-Art documents, specification statements, administrative procedures, design development process descriptions, space planning and design criteria and check lists. Much remains to be done in the direction of more precise and comprehensive communications within the construction industry with measurable performance criteria a mainstay of this goal.

Experience and lessons from an innovative housing project using the performance concept, W. Allen and P. Rich, *SP361, Vol. 1*, pp. 339-344 (Feb. 1972).

Key words: Building systems; education; government sponsored research, need for; housing—industrial, innovated, prototype, low-rise high-density industrialization; performance requirements.

A large low-income project of low-rise construction has been completed in an industrialised building system selected by competitive bidding based upon performance criteria written by the architects. Provisional building designs were prepared in advance as part of an innovative community plan and formed part of the guidance in formulating the criteria. Initial screening reduced the number of bidders to three, all of whom had then to be assisted to develop conformity to the criteria. This part of the project demonstrated the need for whole-dwelling performance requirements established nationally.

Examples are given of the ways in which the design requirements of low-rise high-density development influenced the performance criteria. They are the need to park cars beneath 3- and 4-storey construction, the assembly constraints due to narrow pedestrian passages, a need for stepback balconies and terracing, and party floors which meet fire and sound requirements.

Unconventional performance-based specification items were also exemplified. Concrete finishes were prescribed by Munsell classification, and were also required to deter scribbling. Weather-tightness of joints, thermal performance (in some detail), sound insulation and fire were covered.

The bidding procedure required a new sequence and form for contract documents and this is described.

Prototype dwelling had to be built for agreement on quality of finish and to remove difficulties from the assembly process. Some criticisms are made of the inadequacy of preliminary trials which is unavoidable at this stage as present conventions operate, and this is noted as a cause of some defects which later became evident.

Other lessons are identified. The performance approach requires equivalent development of evaluation and testing procedures, and changes in legal and contractual matters. The vital role of building research organisations for monitoring and feed-back is emphasised for the collective learning process of the professions and industry. The relation between responsibility and deficiencies in the absolute state of knowledge for innovational situations is noted. The educational unpreparedness of the industry is emphasised as a barrier and cause of enhanced risk.

Finally, five major factors of building education and administration which need review by governments promoting innovation are identified.

**Evaluation process of performance and cost as applied to existing housing prior to rehabilitation,** C. Forsberg and G. S. Birrell, *SP361, Vol. 1*, pp. 345-356 (Feb. 1972).

**Key words:** Analysis; cost; evaluation financing; housing; improvements; individual; inspection; minority groups; performance; real world; rehabilitation; synthesis; system; user needs; user values.

This paper presents a process for evaluating the performance of existing homes and planning suitable changes for users who would like to improve this performance. The process was evolved as a result of field research work in aiding minority group families evaluate their homes. The process is intended to enable a housing advisory group assist families in satisfying their individual User Needs. Given that family's home and their priorities for its improvement, income, and available financing, the process derives realistic rehabilitation choices available. Topics discussed include technical/human housing user interface problems, presentation of information, housing requirement analysis process, individual housing user value rating analysis, housing user financial analysis and the organization of the advisory service. This paper maintains a simple level of description and discussion to keep the system uncomplicated enough to operate in the harshness of real-world field work of aiding minority groups rehabilitate their homes.

**Performance specifications for office space interiors,** T. E. Ware, *SP361, Vol. 1*, pp. 357-374 (Feb. 1972).

**Key words:** Building process; building systems; "closed" systems; management; office buildings; "open" systems; performance specifications.

The Public Buildings Service of the General Services Administration, which creates a \$200 million annual market for Federal office buildings, commissioned the Building Systems Section of the Building Research Division of the Institute for Applied Technology, National Bureau of Standards, to conduct an experiment demonstrating the feasibility of the Systems Approach to designing, specifying and constructing complex buildings. Thus, the Government is using its building program for its own benefit while making a public experiment intended to replace prescriptive specifications with Performance Specifications based upon a specific definition of user's needs. This approach will modify—perhaps drastically in some instances—the products, rules, people, resources and energy involved in the building process. It is not intended to supplant the traditional design process or construction process, but rather, it is intended to combine all the elements in the design and construction process to more precisely and efficiently produce a desired result. The principles of this project are examined in such terms that their application to other projects may be expedited.

**Performance requirements for windows,** E. Paulsen, *SP361, Vol. 1*, pp. 375-384 (Feb. 1972).

**Key words:** Air-tightness; performance characteristics; performance parameters; rain-tightness; sealed glazing units; wind loading; window.

A window is defined as any part of a vertical external wall which is predominantly filled by transparent or translucent material and where the primary function of a window is to furnish the adjacent room with sufficient daylight and provide a clear and undistorted view to the outside.

Statements of performance requirements are given under the following headings: Transparency and vision, light transmission, glare, control of solar radiation, thermal insulation and condensation, sound insulation, airing (ventilation), air-tightness, rain-tightness, strength and stiffness, control of opening light, security against illegal entry, fire resistance, escape from fire, appearance, dimensions, durability of operating parts and durability of materials.

**Evaluation of window performance,** A. G. Wilson and J. R. Sasaki, *SP361, Vol. 1*, pp. 385-394 (Feb. 1972).

**Key words:** Performance criteria; performance evaluation; window characteristics; window evaluation; window functions; window requirements; window standards.

Windows are used in the enclosure of buildings to permit entry of natural light, a view of the outdoors, and ventilation. In addition, windows must perform the same function of separating interior and exterior environments as the remainder of the enclosure. Functions related to transparency may be in conflict with those relating to other desired attributes of the building space; this creates the need for considering cost versus benefit on a system basis in establishing performance criteria. This paper deals with the current status of evaluation of windows as environmental separators.

Many aspects of performance cannot be adequately predicted from basic principles, hence a number of standard tests are evolving for evaluation of some of the primary ones. The tests are widely used in product standards, along with relevant criteria, to classify windows and to define certain minimum requirements. Standard test methods, however, have some important limitations in relation to predicting and specifying performance in-use. Some performance characteristics, particularly those involving heat and mass flow, are interdependent although they are usually evaluated independently or are influenced by factors that are excluded or fixed in standard test methods. Where in-use performance of windows is critical, it may be necessary to resort to more complex tests that attempt to take account of all the major factors influencing the final result. This is economically practical only on major construction projects. The development of information to assist the designer in predicting window performance for the majority of situations, utilizing data obtained from standard tests, is, therefore, a desirable goal. The designer will, however, always need to exercise judgment in relating the limited information provided by tests, or other methods of prediction, to the real situation.

**Effect of envelope design on cost performance of office buildings,** M. Anson, W. B. Kennedy, and J. W. Spencer, *SP361, Vol. 1*, pp. 395-406 (Feb. 1972).

**Key words:** Cost analysis; design criteria; external envelope; office building; performance evaluation.

Building design ideally should cover a sufficient range of design alternatives to enable selection of a combination of the performance variables which is as near optimum as can be obtained with the money available. In practice most design variables do not relate simply to the performance variables, and the best that can be done is to check the various performance levels of a design selected on the basis of past experience, amending those features found to be unsatisfactory. This conventional procedure can be improved as much by the development of suitable computational routines as by further refinement of direct measurement of performance.

This paper reports substantial progress with the computation of air-conditioning costs, which when both initial



operating costs are taken into account is the biggest cost item in an office building. The peak air-conditioning load, the sum of the initial costs of the plant, and the envelope plus plant operating, maintenance, and replacement costs over the life of the building have been calculated for 122 variations of a hypothetical building situated in Melbourne (38 °S, 145 °E).

The study showed that the return on investment could be increased from 10 to over 11% for a hypothetical building with 150,000 sq. ft. of rentable space depending on envelope design. For smaller buildings this increase could be even higher because the ratio of the envelope area to volume of the building increases as volume decreases.

Tables and graphs are presented which give some consideration to the relative economic effectiveness of building envelope materials and fenestration.

**Use of modern computer programs to evaluate dynamic heat transfer and energy use processes in buildings,** T. Kusuda and F. J. Powell, *SP361, Vol. 1*, pp. 407-418 (Feb. 1972).

**Key words:** ASHRAE Task Group Energy Requirements; computer application; heating/cooling load; room temperature; thermal environment.

Salient features of the ASHRAE (American Society of Heating, Refrigerating and Air-Conditioning Engineers) Task Group procedures for calculating heating and cooling load are described. It is stressed that the significance of the thermal storage effect is to be found in the conversion of the heat gain process into the cooling load, even in commercial buildings.

An NBS computer program (NBSLD) was used to augment the ASHRAE methodology. This program was designed to predict the indoor temperature of buildings with limited air conditioning or none at all. Various calculation results obtained by NBSLD are illustrated, some of which are compared with the experimental results.

A simple cooling load calculation illustrated in Chapter 28 of the 1967 ASHRAE Handbook of Fundamentals is used to compare the results obtained by the NBSLD program and the program developed by the U.S. Post Office Department (USPOD), which is an adaptation of the ASHRAE Task Group Procedure.

**The application of total energy systems to housing development,** P. R. Achenbach and J. B. Coble, *SP361, Vol. 1*, pp. 419-430 (Feb. 1972).

**Key words:** Energy conservation in housing; energy systems for housing; environmental quality in housing; field study of energy systems; total energy systems; utility system performance.

A pilot investigation of the performance of a total energy system was undertaken by the National Bureau of Standards to evaluate the potential for decreasing the amount of fuel required to provide the utility services to an apartment complex of 500 units and for better control of noise and air pollution. This installation is being made at a site in Jersey City as a part of the BREAKTHROUGH program of the Department of Housing and Urban Development. The selection of the site followed a feasibility study of eleven sites distributed over the United States and the preparation of a performance specification which set forth the design conditions, the requirements for reliability, stability and safety of the system and the environmental quality that must be attained.

The pilot total energy plant is being extensively instrumented to determine its thermal efficiency; the daily and seasonal load patterns; the reliability of the utility services;

the level of noise and pollution control; the maintenance and repair requirements; the owning and operating costs; and the occupant response to his environment.

**A morphological performance evaluation technique for moisture problems in buildings,** J. Saarimaa, *SP361, Vol. 1*, pp. 431-449 (Feb. 1972).

**Key words:** Building moisture problems; effects; evaluation; morphological research; movement; sources.

The paper gives a picture of an evaluation technique which may be suitable in solving moisture problems of buildings. The final goal of the procedure is the setting up of the performance requirements which are needed for building elements and products in order to ensure the expected performance of constructions. The evaluation is done with the help of a matrix which is built up as follows: The problem may be divided in the following main factors:

1. Moisture sources
2. Moisture movement and fixation
3. Effects of moisture
4. Performance requirements

Each factor will then be given all the possible values it can get in reality. The main factors form the first vertical column of the matrix, and the possible values of these factors are put on the horizontal lines. The principles and the procedure of the evaluation technique will be discussed. The values of the various "factors" will be introduced, and examples given on the results obtained.

**Sizing of water heating equipment,** L. G. Spielvogel, *SP361, Vol. 1*, pp. 451-463 (Feb. 1972).

**Key words:** Domestic hot water systems; hot water heating; hot water system design; hot water usage; survey of hot water use.

This paper contains the results of studies made on 162 buildings throughout the U.S.A. to determine the nature of hot water use in order to establish design criteria for sizing water heating equipment in various types of buildings.

An extensive search of the literature was conducted and analysed, and there is an extensive bibliography and list of references on this subject available.

Meters were installed in the cold water inlet to water heating systems and hourly readings were taken for periods of up to 1 1/2 years. Data was collected and organized in 10 categories of buildings, men's college dormitories, women's college dormitories, motels, nursing homes, office buildings, food service facilities, apartment houses, elementary schools, junior high schools, and high schools. Test data was analyzed with respect to peak hourly, daily and average flow rates in order to compare with previously available information. Further analysis was done on multiple-hours use of hot water, and curves were drawn representing an infinite number of relationships between storage capacity and recovery capacity, any of which will adequately meet the requirements for hot water in each type of building.

Some of the factors that influence hot water consumption are discussed. The influence that hot water temperature has on demand and consumption is analyzed. New definitions are developed for efficiencies in connection with water heating systems. Limited information on energy consumption of water heating systems is discussed. Safety factors are recommended. There is some discussion on instantaneous flow rates based on data extrapolation.

Typical profiles for each category of building are shown with hour-by-hour flows for the day in which the peak hourly demand occurred, the day in which the peak daily de-

mand occurred and the hour-by-hour average of all test data for the particular building selected.

With this information it is now possible to make an economical selection of water heating equipment, based on both first cost and operating cost. Comparing the recommended sizing methods with those methods previously used shows a significant reduction in both storage capacity and recovery capacity for most types of buildings.

**The development of performance criteria and test procedures for the piping of sanitary drain, waste and vent systems in residential service,** R. T. Holtz, *SP361, Vol. 1*, pp. 465-476 (Feb. 1972).

**Key words:** Criteria for DWV pipe; drain, waste, and vent systems; environmental factors; evaluative methods for DWV pipe; thermoplastic pipe.

The development and use of new plastic materials for drain, waste and vent piping emphasized the need for the identification and definition of service requirements to be used as a basis for minimum performance criteria for these products. Such criteria would have to take account of all of the pertinent application and service factors to which a typical DWV product might be exposed, and to provide for safe and satisfactory performance under these conditions for the projected life of the building. The availability of such criteria would enable the development of materials and the design and engineering of DWV products to more accurately meet the needs of this plumbing service. It would also facilitate the design and evaluation of systems fabricated from various materials.

Several years ago, a task force was established under the auspices of Standards Committee A112 of the American Standards Association (now American National Standards Institute—ANSI) to:

1. Determine the service criteria for residential drain, waste and vent systems;
2. Establish the design criteria and test conditions for plastic DWV materials to meet the service requirements.

The task force, composed of experienced sanitary engineers and others knowledgeable in plumbing engineering identified the following general categories of service criteria: Chemical, Mechanical, Thermal and Environmental. Objective minimum or maximum conditions for each of these criteria in these categories were determined, and test conditions were recommended, based on an assumed fifty year usage.

Following completion of the service criteria, the group determined test procedures, simulating end use conditions and established design criteria consistent with the minimum service criteria for DWV systems. This paper emphasizes the methods used in the study, the service conditions identified as pertinent to DWV exposures, and the criteria established. It then discusses how these criteria were adapted to facilitate adequate performance through appropriate design of plastic DWV piping.

**Simplified acoustical measurement procedures for building code enforcement,** M. J. Kodaras, *SP361, Vol. 1*, pp. 477-481 (Feb. 1972).

**Key words:** Acoustical field measurements; building code enforcement; noise control enforcement; noise control in dwellings.

New and revised building codes now contain specific requirements for acoustical privacy in multifamily dwellings. These performance specifications for sound transmission loss, impact sound insulation, maximum per-

missible sound power radiated by mechanical equipment and isolation of structural vibration sources must be subject to field measurements to assure compliance with the building code provisions. In most cases the results of these field measurements need only indicate a "pass" or "fail" result.

This paper reviews some of the simplified field test procedures now in use and in process of development.

**The effect of illumination systems upon visual performance,** I. Lewin and J. W. Griffith, *SP361, Vol. 1*, pp. 483-490 (Feb. 1972).

**Key words:** Illumination systems; lighting; performance concept; task contrast; veiling reflections; visual performance; visual task.

One of the critical human factors in building design is the provision for an adequate level of visual performance, in relation to the speed and accuracy of vision. It has only recently been recognized fully that the amount of illumination on a visual task may be of secondary importance to that of another variable, the "task contrast." The concept of "Contrast Rendition Factor" will be developed, where the amount of contrast produced on a written task by any given illumination system may be evaluated in relation to a reference standard. Recent researches will be reported which indicate the ineffectiveness of present conventional illumination systems.

Further research undertaken in the development of unconventional systems of illumination will be reported, and it will be shown that a unique distribution of light within a working area can produce very substantial visual performance increases, without increasing the electrical input to the system.

Whereas the paper will include some theoretical concepts in relation to visual performance, its chief purpose will be to provide practical guidelines for the improvement of this factor.

**The performance concept in the service of technical evaluations of building innovations,** D. E. Dobson, *SP361, Vol. 1*, pp. 491-502 (Feb. 1972).

**Key words:** Agrément; durability prediction; economic aspects; evaluative judgement; need for clarity of purpose; performance concept; plastics in fire; rain penetration; robustness of construction; technical evaluation; uniformity of assessment; weathering.

The introduction gives a broad picture of the increasing effort of the National Building Research Institute (NBRI) in the field of technical evaluation and performance requirements. Terminology is also defined. This is followed by a section in which work on certain selected aspects of performance is discussed. The concluding sections deal generally with the performance concept and its cardinal position in the evaluation of innovations in building, and bring out some of the practical limitations of the concept and the continuing need for the exercise of evaluative judgement.

**Technical evaluation of components: agrément,** G. Blachère, *SP361, Vol. 1*, pp. 503-506 (Feb. 1972).

**Key words:** Agrément; assessment; durability; new materials; new processes.

It is a problem for a builder to know whether a component presents the physical properties which are needed for it to play its part correctly in the finished whole.

Various means are available to give this proof:

—the use of science and exact physical measurements,



- the use of traditional knowledge recorded in codes of practice and standards,
- the direct proof by performance tests.

Unfortunately among the properties required is durability and often it may not be possible to test it by one of the preceding methods, because scientific knowledge may be lacking, experience does not exist for new components, and performance testing takes too long where durability is concerned. Nevertheless it is necessary to have, if not a proof, at least a judgement about the durability of new materials, components, and building systems, and if a completely logical proof is not possible, the advice of the best experts based on a broad examination and various tests is the best that can be found. Such is the *agrément* procedure. People such as manufacturers, builders, and administrative authorities needing the best advice on the durability of new things, can ask for an *agrément* issued by a group of experts drawn from all parts of the building field, utilizing the results of measurements of natural or semi-natural tests on a full or reduced scale, and experience with short term use.

It is possible to draw up a check list of the various properties that may be required of an element in service and of the means of testing them. Some examples of such properties and tests will be given.

For convenience of the users of *agrément* a control of the manufacture of approved products is possible and may be indicated by a mark.

An *agrément* procedure is used in all the Western European countries which belong to the UEAtc, and which cooperate in writing common directives for *agrément* and in recognizing each other's *agrément* certificates.

**Performance requirements in a systematic method for selecting building materials**, K. Shirayama, K. Imaizumi, K. Kamimura, K. Kondo, F. Saito, T. Nireki, K. Ito, F. Tomosawa, S. Sugawara, H. Suzuki, K. Kawase, Y. Takahashi, S. Oka, Y. Mimura, M. Ito, *SP361, Vol. 1*, pp. 507-518 (Feb. 1972).

**Key words:** Building; classification; comparison; elements; materials; performance requirements; selection.

The purpose of the study on "Systematic Method for Selecting Building Materials" is to establish a system or rational method for solving the problem of how to select and how to use building elements or materials. This selection system is composed of the following steps:

1. Identify the conditions concerned with the use of building elements or materials and put them in order. These conditions are named "Given Conditions."
2. Select necessary performance requirements for the buildings or components according to the "Given Conditions."
3. Transform performance requirements of the building to those of building elements or materials.
4. Evaluate performance or properties of existing building elements or materials based on the results obtained by suitable proposed methods of tests, calculation, and so on.
5. Select building elements or materials by means of comparing their evaluated performance or properties with those required.

The outline of this systematic selecting method is presented putting stress on the following points.

- a. Classification and arrangement of the performance requirements.
- b. Selection of necessary performance requirements according to the "Given Conditions."

c. Relation and transformation between the performance requirements of different levels.

**Proposed method of test for evaluating performance of buildings, building elements, and materials**, K. Shirayama, K. Imaizumi, K. Kamimura, K. Kondo, F. Saito, T. Nireki, K. Ito, F. Tomosawa, S. Sugawara, H. Suzuki, K. Kawase, Y. Takahashi, S. Oka, Y. Mimura, M. Ito, *SP361, Vol. 1*, pp. 519-529 (Feb. 1972).

**Key words:** Building elements; building materials; evaluation; performance; performance requirements.

In order to select suitable building elements or materials rationally, it is essential to make clear their performance corresponding to the requirements. To achieve this, fifty standard testing methods, with evaluating methods of test results, were prepared.

These testing methods are classified into the following three groups:

- a. Tests for materials (Materials-related tests)
- b. Tests for building elements (Building element-related tests)
- c. Tests for space or building (Space or building-related tests)

In each testing method, the following items are included.

1. Designation of testing method with its classification symbol.
2. Relevant performance requirements.
3. Scope
4. Test specimen description
5. Procedure
  - 5-1 Outline
  - 5-2 Apparatus
  - 5-3 Conditioning prior to test
  - 5-4 Details
6. Evaluation method and grade determination
7. Report
8. Notice, other relevant testing methods.

Titles of all proposed methods are tabled and some of them are referred to in detail.

**Performance of components with special attention paid to the practical implementation**, G. Christensen, *SP361, Vol. 1*, pp. 529-534 (Feb. 1972).

**Key words:** Components; dirt repelling; evaluation; feedback; open system; performance requirement; scratch resistance; testing; water-spray repelling.

It is explained how the use of the Performance concept on the level of components has an open building system as a prerequisite and further that a number of compatibility problems thus must be solved.

Manufacturers and designers have a common need in describing the attributes offered or required by a component on a Performance base. An example of the basic principle for such a common Performance language is shown.

The principle is used for describing the Performance attributes for bathroom walls regarding scratching resistance, ability to repel dirt, and ability to reject water spray. The background for the use of these tests is also discussed.

It is finally underlined how important it is to explain to the building industry that the Performance concept is created as an invitation to new technical solutions within building and it is not meant as a new set of restrictions to be used instead of traditional building regulations.

**Increasing the application efficiency of performance tests with analytic procedures**, S. K. Suddarth and D. H. Percival, *SP361, Vol. 1*, pp. 535-543 (Feb. 1972).

**Key words:** Analysis and performance tests combined; computerized analysis; plane frame structures; test results; use of structural analogs.

A method is illustrated for combining more advanced analytical procedures with performance tests of plane frame structures. A fundamental part of the method is the development of an analog, or mathematical model, of the real structure. This analog, which may be as simple or as complex as the situation warrants, is processed by a computerized system to produce a complete structural analysis. In use, performance tests of parts of the frame, particularly joints, can be used to evaluate needed parameters in the analog of the entire structure.

Three quite different examples are given showing how the analog reproduces the deformation patterns corresponding to the full-scale test structures. Acceptance of internal stresses in the analog as sufficient estimates of internal stresses in the prototype is based primarily on the deflection correspondence.

The possession of a suitable analog permits examination of a wide variety of structural variations and load cases that require verification with only a relatively small number of prototype tests.

**Evaluation of structural concrete members penetrated by service systems, J. M. Hanson, W. G. Corley, and E. Hognestad, *SP361, Vol. 1*, pp. 545-556 (Feb. 1972).**

**Key words:** Analysis; concrete beams; concrete plates; ducts; openings; serviceability; strength; structural performance; tests.

Performance requirements for structural concrete members containing openings are defined. Both strength and serviceability are considered. Results of tests carried out by the Portland Cement Association to evaluate performance of flat plate and beam and slab floors containing embedded metal ducts and of concrete joists with holes in their webs are described.

**A performance approach to the design of fire-resistive buildings, L. G. Seigel, *SP361, Vol. 1*, pp. 557-566 (Feb. 1972).**

**Key words:** Building design; fire protection; fire resistance; fire-resistive buildings; structural design.

For many years, fire-endurance requirements for building structures and fire-insurance rate schedules for buildings have been based on performance demonstrated in standard fire tests. However, many conditions that may be encountered in an actual building, such as structural restraint, and partial or nonuniform fire exposure are in no way covered by standard fire test procedures. Therefore, the results of standard fire tests (as presently defined) may not represent the performance to be anticipated in a building. The structural performance of a building during a fire depends on the temperatures reached by the structural members of the building independent of how such temperatures are attained. Therefore, an analytical approach to the determination of fire resistance should be considered based on appropriate temperature limits for the structural materials of the building. Fire-resistive design may then be accomplished by providing adequate thermal protection to the structure so that the temperature limits of the structural materials will not be exceeded.

**The resistance of brick walls to lateral loading, H. W. H. West and H. R. Hodgkinson, *SP361, Vol. 1*, pp. 567-576 (Feb. 1972).**

**Key words:** Brickwork; experimental; lateral loading; performance; research; residential structures; safety; structural masonry.

The Building (Fifth Amendment) Regulations 1970 lay down performance requirements to prevent progressive collapse, following and incident, in buildings of 5 storeys or more. Essentially either the building must be so designed as to provide alternative paths of support in the event of the removal of a main structural member, or the members must be designed to withstand a lateral load of 5 lbf/in<sup>2</sup>. Laboratory tests to determine the lateral strength of various types of brick wall are briefly described and the application of the results to the evaluation of the performance of real buildings discussed. It is concluded that solid brick walls more than 7 in. thick may be "deemed to satisfy" the requirements of the Fifth Amendment.

**Experimental gas explosions in load-bearing brick structures, N. F. Astbury, H. W. H. West, and H. R. Hodgkinson, *SP361, Vol. 1*, pp. 577-592 (Feb. 1972).**

**Key words:** Building structures; damage; gas explosions; limiting pressures; load-bearing brickwork; venting.

The resistance of normal types of fenestration and cladding, masonry walls, and a full-size load-bearing brickwork structure to explosions of town gas/air and natural gas/air mixtures was determined. The explosions were generated by igniting stoichiometric gas-air mixtures in balloons, or layered mixtures in the explosion space. Peak pressures were recorded by transducers. Explosion damage to the structure is discussed. Normal windows and cladding failed at pressures below 1 lbf/in<sup>2</sup> and in so doing provided venting relief limiting the maximum pressure developed, in accord with a simple formula. Under a precompression of about 30 lbf/in<sup>2</sup> a cavity wall will crack at about 3.3 lbf/in<sup>2</sup>. A 4 1/2 in. wall fully restrained by returns failed at about 5 lbf/in<sup>2</sup> and a 9 in. wall fully restrained cracked but did not fail at 15 lbf/in<sup>2</sup>. In a normally vented simulation of a full-scale real domestic situation, it was not possible to raise an explosion pressure greater than just over 3 lbf/in<sup>2</sup>. Possible amplification of explosion effects due to cascade or turbulence in interconnected rooms is briefly discussed and will be studied further.

**Performance characteristics for timber frame joist floors, H. Hansen, *SP361, Vol. 1*, pp. 593-600 (Feb. 1972).**

**Key words:** Deflection (floors); dwelling; floor (wood); joists; loads; performance criteria; strength (floors); vibration (floors).

Different loads which act on a floor are discussed and a factor of safety based on economic criteria is used. The paper also discusses vibration and deflection criteria for timber frame joist floors.

It is pointed out that the deflection under a single point load may be used as a performance criterion for human perception to initial vibration.

An acceptable strength and deflection performance of a wood-joist floor system is given.

**Performance requirements for floors, C. Bring, *SP361, Vol. 1*, pp. 601-612 (Feb. 1972).**

**Key words:** Colour fastness; flatness; flooring; indentation; performance requirements; properties; quality classes; rolling load; surface evenness; test methods; warmth to touch.

Several properties of floors and floorings have been studied. Test methods have been used which allow com-



parisons between different types of floor materials and floor constructions. On the basis of tests on actual floors and in the laboratory, classified performance requirements are proposed.

The validity of the properties for different floorings and subfloors is considered. Typical quality classes of actual floors are surveyed. Suggestions for performance requirements for the discussed properties of floors in dwelling-rooms are made by way of an example.

With the users' requirements and the future conditions in mind, relevant performance requirements can be chosen for different projects with the help of the paper. The intended quality of a floor can generally be obtained in more than one way. However, none of the alternatives fulfills all requirements. Extremely high requirements on certain properties often must be combined with low requirements on other properties for the same floor. Already extremely high requirements on two antagonistic properties—like resistance to indentation and warmth to touch—might result in the elimination of almost all floors or floorings.

**Performance analysis of floors**, J. Saarimaa, Tenho Sneek, and M. Wäänänen, *SP361, Vol. 1*, pp. 613-623 (Feb. 1972).

**Key words:** Classification of floors; evaluation of floors; external factors; floorings; floors; performance analysis; properties of floors.

The paper discusses the main principles, which may be used in setting up performance requirements for floors. Performance requirements, which define the performance of a floor may be derived from an analysis of the external factors, which affect a floor in use by juxtaposition of the external factors and the properties of the floor. The following levels of building are considered in the analysis: space, building element, product combination, product, material. The analysis of external and internal factors as well as the relation between external and internal factors has been carried out on these levels. An evaluation technique, which could be used for selection and development of floors and floorings has been developed. The method is based on the identification and classification of the external factors, classification of rooms, listing of requirements and classification of rooms according to the requirements. The main purpose of the paper is to give an example of how the ideas of performance analysis could be applied to floors.

**Strength criteria of glued-laminated timber**, B. Bohannan, *SP361, Vol. 1*, pp. 625-632 (Feb. 1972).

**Key words:** Defective material; design criteria; design stresses; glued-laminated timber; knots; lamination; lumber grades; prestressed wood; slope of grain; strength criteria; strength ratio; strength-reducing characteristics; structural.

Accurate knowledge of the properties of any engineering material is essential to its proper uses. Recognizing this fact, the U.S. Forest Products Laboratory has had a continuing research program to better define the strength characteristics of glued-laminated construction, a versatile engineering material. Early research in the 1930's was the foundation for the glued-laminated industry in the United States. Design and manufacturing criteria were developed based on glued members which were relatively small by today's standards. With industry growth, manufacturing techniques and architectural design developed to the extent that timbers of almost unlimited size and shape were possible, but engineering technology did not keep pace. However, an extensive research effort during the 1960's has developed related engineering technology for the large timbers. This research established the effect of several factors

involving strength and design of large timbers—a principal one being the effect of tension lamination quality on beam strength. Such research has resulted in revised specifications for glued-laminated timbers which will insure a more reliable engineering material.

**Performance requirements for mechanical fasteners used in building**, E. G. Stern, *SP361, Vol. 1*, pp. 633-642 (Feb. 1972).

**Key words:** Bolts; building assemblies; building components; building constructions; framing wood; improved nails; mechanical fasteners; mechanical fastenings; nails; screws; staples.

The selection of mechanical fasteners used for joining and fastening of materials, assemblies, and components is influenced by a variety of criteria, all of which are related directly to the anticipated performance of the assembled items. The mechanical fasteners need to be selected on the basis of their actual and economic availability, versatility, applicability, physical and mechanical properties, rigidity and damping capacity, compatibility, thermal properties, fire resistivity, reliability including their resistance to creep, maintenance and repair of the finished product, and feasibility of testing for performance evaluation and performance predictability. These performance criteria are given detailed consideration in order to facilitate the writing of performance specifications covering mechanical fasteners as well as mechanical fastening in building constructions. Whereas the subject matter is approached from the overall viewpoint, reference is made to a few selected specific applications in order to draw attention to the importance of the performance concept under given conditions.

**Performance criteria for composites in building**, A. G. H. Dietz, *SP361, Vol. 1*, pp. 643-651 (Feb. 1972).

**Key words:** Classes of composites; composites for building; evaluation; performance criteria; performance statement.

Composite materials for building are mainly particulate, fibrous, or laminar. Examples are to be found in buildings in various parts of the world. Performance criteria are especially pertinent because composites are frequently put together to meet specific situations. Great care is needed to make sure that the criteria accurately reflect requirements. A statement of performance criteria is of little value, unless the actual performance of a composite building component can be tested. Some tests are equally applicable to composites and to other materials, but others are specific for composites. They include, for example, the character of the bonds among constituents; the fire behavior of a composite, especially penetration, flamespread, and smoke evolution; the combined mechanical behavior; and durability. New types of tests, such as ultrasonic evaluation of bond, are needed in many instances. Standard tests may require adaptation for evaluation of composites.

**Basic problems and conditions of long term performance of materials and structures**, O. Valenta, *SP361, Vol. 1*, pp. 653-668 (Feb. 1972).

**Key words:** Capillary elevation (head); coefficient of permeability; kinetics of deterioration; open pores; steady and unsteady flow; tests of absorption, permeability and capillary elevation.

Appropriate choice of materials for structures of all sorts must be based on their properties and long term performance in specified conditions of their application. Besides the main mechanical physical factors, factors con-

cerned with the pore system in relation to the possibility of water or gas penetration must be considered as basic properties in the study of long term behavior of any material in natural weathering or other conditions. Actual state of standards concerned with humidity and water permeability of materials is analysed. Absorption, permeability and capillary elevation are considered as the main characteristics of materials.

Absorption test—its purpose and methods are discussed in the light of the mechanics and kinetics of water penetrating into a porous body. Some standards British, Russian, American and Czechoslovak are then quoted and analysed as to their interpretation and compliance with the need to describe the pore system effectively. The need of scientific base of such tests is stressed.

Permeability test—its purpose and methods are given with special emphasis to the need of providing us with the coefficient of permeability. British, Russian, German and Czechoslovak standards for testing are then surveyed from this point of view.

Capillary elevation test in relation to the importance of the capillary elevation head is analysed and Czechoslovak standards are quoted.

Mechanics and kinetics of water permeation into materials, its factors and their determination are considered as to their effect and importance for their performance in structures. Both steady and unsteady flow of water are considered in relation to the determination of the coefficient of permeability. Capillary properties of the pore system should be provided by test. The importance of these characteristics for the analyses of tests as well as of practical cases is then stressed by cases of practical application.

**Pore properties in the evaluation of materials**, J. M. Haynes and Tenho Sneek, *SP361, Vol. 1*, pp. 669-675 (Feb. 1972).

**Key words:** Materials; performance evaluation; pore size distribution; porosity; specific surface.

Many technologically-important materials are porous, and can be characterised by such pore parameters as porosity, specific surface and pore size distribution. The pore structure of such materials often plays a dominant role in controlling their useful properties. Attention is therefore drawn to some of the difficulties to be encountered in performance evaluation of such materials, when measured pore parameters have to be taken into account.

**The definition of a low intensity fire**, D. Gross and J. B. Fang, *SP361, Vol. 1*, pp. 677-686 (Feb. 1972).

**Key words:** Buildings; calorimetry; combustibility; fire intensity; flame spread; furnishings; heat release; thermal radiation; wastebaskets.

A reproducible fire of low intensity may be used for the realistic performance evaluation of interior finish materials and of structural building elements. The burning behavior of furniture and the contents of wastebaskets are defined in terms of the rates of heat release, heat transfer to the surrounding walls, and heat losses by radiation and convection. Experimental measurements of temperature and radiation levels within a room are summarized for a variety of combustible contents and mass loadings. Selected low intensity fires have been examined for repeatability and for potential use in evaluating fire safe requirements for interior finish materials in terms of the spread of flame, generation of smoke and overall fire growth pattern.

**The interaction between mortar and masonry units as a basis for standards for masonry mortars**, Tenho Sneek, *SP361, Vol. 1*, pp. 687-692 (Feb. 1972).

**Key words:** Fresh mortar; interaction between masonry mortars and units; masonry mortar; mortar evaluation; mortar standard; suction of masonry unit; winter masonry.

The paper describes a draft standard for masonry mortars which is based on the application of the performance concept on the "product" (material) level. The approach is based upon a statement that the solutions have to give optimal service, under the action of the external factors. In this case, the object of the analysis is fresh mortar. The most important external factor affecting the mortar is the suction exerted by the masonry units. The removal or non-removal of water has deciding effects on the mortar joint as a whole. Therefore, the properties of the mortar have to be matched to the properties of the unit. The evaluation of the mortar is based on the interaction of the mortar and the masonry unit. Testing methods and the general background of the evaluation are described. The final evaluation lies in the hands of an expert panel.

**A performance evaluation of thin bed adhesive mortar in concrete masonry construction**, L. A. Kuhlmann, *SP361, Vol. 1*, pp. 693-709 (Feb. 1972).

**Key words:** Adhesives; concrete masonry; cost performance; ground concrete block; mortar.

The rising cost of labor in recent years has prompted the concrete block industry to develop new methods of building walls. Of the many techniques created, the concept of gluing together dimensionally accurate concrete units has been the most successful. For the past 10 years, projects have been built with an adhesive mortar and block, providing an arena for demonstrating the performance characteristics of this concept. Both physical properties from ASTM test methods and economics from case histories prove that this concept is acceptable and practical.

**Performance requisites for concrete building components and their achievement with gap-graded concrete**, S. Li, D. A. Stewart, and V. Ramakrishnan, *SP361, Vol. 1*, pp. 711-718 (Feb. 1972).

**Key words:** Aggregate grading; cement content; concrete construction; creep; durability; economy; gap-grading; shrinkage; strength; structural concrete.

Performance requirements for all reinforced and prestressed concrete building components are established and criteria for evaluating such performance requirements are given. Their achievement with gap-graded concrete is substantiated with experimental results and field observations.

**Relating materials quality to materials performance to structural performance of concrete**, B. Mather, *SP361, Vol. 1*, pp. 719-724 (Feb. 1972).

**Key words:** Aggregates; cement; concrete; concrete quality; materials; performance; portland cement; structural performance.

Portland cement, aggregates for portland-cement concrete, admixtures for concrete, and curing materials for concrete are usually procured for use in construction under specifications that stipulate levels of quality as indicated by the results of standardized tests of samples. The information obtained from these tests is believed to be related directly or indirectly to levels of performance of the material itself, the composite of which it is a constituent, the structural element of which it is a component, and the structural system of which it is an element. The testing is limited to determinations that can be completed in the time available for testing



and at an appropriate cost. The levels of quality are selected to be few for simplicity and are frequently higher than needed to insure adequacy of performance in the specific situation; rarely lower. Attention has primarily been directed to those few cases where less than adequate performance has resulted. Greater economies and more prudent utilization of natural resources will result if attention were directed to those much more numerous cases where stipulated levels of quality are higher than needed.

**Proposed method for prediction of corrosion of reinforcement in concrete**, J. Saarimaa, *SP361, Vol. 1*, pp. 725-732 (Feb. 1972).

Key words: Concrete; corrosion; durability; material properties; morphological research; performance analysis; reinforced concrete; reinforcement.

A performance evaluation technique suitable for the evaluation of corrosion of reinforcement in concrete is explained. The durability of the reinforcement is a consequence of the combined effects of the environment, the properties of the concrete and the reinforcement, and of the processes caused by the external factors which affect steel concrete. In order to be able to solve the complicated problem a systematical method of evaluation is needed. The prediction could be made with the help of a matrix which consists of a list of all the important factors affecting the corrosion of reinforcement. The evaluation can give both qualitative and quantitative information on corrosion. The evaluation technique is feasible for evaluation of the probability of corrosion of reinforcement in a defined construction. It can also give information on how a construction should be dimensioned in order to avoid corrosion of reinforcement.

**The performance concept applied to building materials—an unattainable ideal**, F. A. Blakey and K. G. Martin, *SP361, Vol. 1*, pp. 733-740 (Feb. 1972).

Key words: Building materials; concrete; functions in building; material prescriptions; performance concept; plastics; property tests.

The performance concept is the only logical basis for building regulations for the selection of building systems and for the whole design process, which does not implicitly restrict the designer on his choice of materials and form. Nevertheless, experience has shown that it remains an impractical ideal when one attempts to apply the concept to specification and control of materials. This is probably most evident for concrete and for plastics, two materials which are discussed in this paper.

There is no dearth of tests for concrete which may be used to assess the performance of the material in various ways, but there remain many important properties for which it is impossible to specify rational limits for the properties measured. There are also many tests which produce results, but these measures are of little value because they are obtained in conditions which are too far removed from the practical conditions in which the material will be used. Shrinkage and standard crushing tests for concrete are considered as examples of these viewpoints and yet might appear to be successful and valid applications of the performance approach.

Plastics may also be characterized by a variety of tests relating to many chemical and physical properties, and being manufactured to meet certain of these properties would also appear to offer opportunity for control by specifications based upon performance tests. However, the functions most frequently required of plastics in building application include aesthetics, weathering, and fire resistance; and the

development of performance specifications to encompass such properties is shown to encounter problems at every step.

In view of these and other examples to be cited, it is proposed that there should be a widespread return to prescription specifications to complement quality and valid performance property testing. The tests needed to police a prescription specification are usually simpler and quicker to carry out than performance tests and are equally satisfactory for control of uniformity.

**Evaluation of performance of materials performance and dimensional stability of resin binders**, K. Gamski, *SP361, Vol. 1*, pp. 741-750 (Feb. 1972).

Key words: Adhesion; composites; dimensional stability test; fillers; performance; resin binders.

Although there are standard methods for evaluating the performance of composites based upon traditional binders such as hydraulic or bituminous binders, we have no methods for evaluating binders and composites made of resin.

The author describes some tests capable of being used and possibly standardized, among which is the dimensional stability measurement test. This test could be adapted to resin binders and composites on one hand, and on the other hand, adapted to large dimensional elements both prefabricated and constructed on site.

**Natural and artificial weathering performance of rigid polyvinyl chloride (PVC) and other plastic materials**, H. F. Stedman, *SP361, Vol. 1*, pp. 751-760 (Feb. 1972).

Key words: Atmospheric pollutants; color—difference and representation; impact resistance; plastics; rigid polyvinyl chloride (PVC); test methods; ultraviolet (UV) radiation; water vapor; weathering—artificial and natural; yellowing.

Rigid polyvinyl chloride and other synthetic plastics as exterior building materials are relatively new, but their use, fabrication and distribution are well-documented. Weathering performance of these materials is taking time to evaluate because of the wide range of variables involved, the general inertness of the substances and the lack of knowledge of the proper test parameters to use. An artificial weathering test method has been developed which takes into account the vital role of moisture in the degradation of plastics. Dual consideration is given to the deleterious effects of ultraviolet radiation alone. Many of the results of this combined method of evaluation have correlated well on an accelerated basis with outdoor performance. The efficacy of outdoor weathering emphasizes the need for a closer examination of UV radiation sources and test atmospheres. Color and surface changes are followed during weathering, and measures of stability are expressed as color difference units and gloss variations. Color acceptability may be evaluated by means of color triangulation. Changes in impact resistance in rigid PVC are as important as the influence of atmospheric pollutants during the natural weathering process. Both phenomena require duplication artificially with the hope of determining time equivalence between the two media.

**Evaluation of structural adhesives for use in housing systems**, T. W. Reichard, L. W. Masters, and J. H. Pielert, *SP361, Vol. 1*, pp. 761-775 (Feb. 1972).

Key words: Accelerated aging; adhesives; bonded structures; durability; glass fiber reinforced plastics; housing systems; Operation BREAKTHROUGH; paper honeycomb; performance criteria; structural sandwich.

As a result of the structural evaluation procedures developed for the "Operation BREAKTHROUGH" program, critical factors occurring in adhesive bonded structural assemblies were identified. The effects of aging, sustained-loading and adverse environmental conditions on these bonded areas were evaluated using small test specimens.

Typical results from this evaluation on two BREAKTHROUGH systems are presented. The results indicate that the accelerated aging procedure used here has a deteriorative effect on the strength of these systems. However, the magnitude of this effect was not judged to be great enough to reduce the strength of the final design below that required by the application. The results presented also show that the effects of adhesive thickness, temperature and sustained loading can be very significant and must be fully considered in design and structural evaluation.

**Performance requirements for bituminous roofings, A. J. Hoiberg, SP361, Vol. 1, pp. 777-787 (Feb. 1972).**

**Key words:** Bituminous; cost; durability; performance; roof behavior; roofing.

Factors related to performance of the shingle and the built-up membrane bituminous roofings are discussed under the general headings of durability, roof traffic considerations, appearance and economic evaluation. Durability relates to resistance to weather including wind and hail, and ability to withstand stresses within the membrane such as caused by thermal and moisture changes and by differential membrane and deck movements. Additional testing of roofing systems for ability to withstand movements is suggested and research methods which seem adequate are cited. Testing and requirements for fire resistance and hazard are described. Model analysis and testing are suggested to determine parameters and properties of materials required to be able to design properly performing traffic decks. Appearance is a primary design consideration for strip and individual shingles, whereas membrane systems mostly are applied for protection only. If a non-black appearance is desired, surfacing of the membrane with aggregate or a coating is feasible and additionally can improve durability. A method of economic analysis to determine the annual cost of a roof over its projected life is proposed. This includes in addition to first cost and annual capital charge, terms for maintenance, and the cost of surface renewal modified by a present worth factor. Quality control of the component parts and in application are key factors, once an adequate design of a roof system has been determined. Bituminous roofs can be varied greatly in design, and with proper care in construction will provide long time satisfactory performance at minimum cost in comparison with other systems.

**Abrasion test and wear resistance of concrete terrazzo flooring tiles, I. Soroka, SP361, Vol. 1, pp. 789-797 (Feb. 1972).**

**Key words:** Abrasion test; Böhme machine; concrete terrazzo flooring tiles; DIN 52108; wear resistance.

The paper summarizes a series of tests, in which the reliability of the Böhme abrasion machine (DIN 52108) in evaluating the wear properties of terrazzo concrete tiles was investigated. In view of the performance of such tiles under service conditions it was concluded that this procedure is not always reliable. It was therefore suggested that the acceptance procedure of such tiles should not be limited to an abrasion test but should also specify a minimum cement content in the terrazzo course. This minimum cement content should be 450 kg. per cu.m while the maximum amount of abrasion should not exceed 1.8 mm.

**Performance tests for finish floors state-of-the-art, W. C. Wolfe, SP361, Vol. 1, pp. 799-806 (Feb. 1972).**

**Key words:** Carpets; cleanability; conducting; durability; flooring; indentation; resilience; slip resistance; static charge; test methods; water resistance; wear.

The need for performance standards in buildings and in finish flooring is recognized but performance requirements and criteria need to be established. Requirements for finish flooring, based on user needs, were divided into three categories in a symposium at the 72d Annual ASTM meeting. These were Health and Safety; Comfort, Convenience and Efficiency; and Economics. Criteria are dependent on the art and science of testing.

Sanitation factors, such as *cleanability* and *air pollution* are difficult to define. Statistics show a number of deaths and injuries from falls but the number of accidents due to *slippery floors* is unknown. *Fire safety* is not discussed as this is outside the scope of our work.

In the second category, *resistance to the movement of wheeled vehicles* is a problem with carpet but not with other types of finish floors. One question about *resilience as related to foot comfort* is whether this is related to fatigue or to foot problems. *Water and solvent resistance* is a problem in certain areas, such as bathrooms, kitchens, and industrial locations. The question of *noise or acoustics* is outside our scope.

*Wear and durability* is related to economics as it is a determining factor in life-cost. Since finish flooring is judged on appearance as well as function, it is important to consider change of appearance in wear testing as well as actual loss of material or wearing through.

The state of the art in test development is reviewed and exploratory work at NBS is presented in the areas of cleanability and stain resistance; slip resistance; indentation and resilience; static charge and conductivity; water resistance; and durability or wear.

**SP361. Volume 2. Performance concept in buildings.** Opening addresses, rapporteur reviews, and discussions. Proceedings of a symposium jointly sponsored by the International Union of Testing and Research Laboratories for Materials and Structures (RILEM), the American Society for Testing and Materials (ASTM), and the International Council for Building Research Studies and Documentation (CIB), Philadelphia, Pa., May 2-5, 1972, B. E. Foster, Editor, Nat. Bur. Stand. (U.S.), Spec. Publ. 361, Vol. 2, 169 pages (Sept. 1972).

**Key words:** Buildings; components; design procedures; experience in use; materials; performance evaluation; performance requirements; user requirements.

Volume 2 records the proceedings of the Joint RILEM-ASTM-CIB Symposium on the Performance Concept in Buildings which was held in Philadelphia on May 2-5, 1972. Volume 1 contains the 82 papers accepted for the Symposium and was published prior to the meetings. This second volume contains the opening addresses; the reports of the rapporteurs, which include a review of the papers and a general discussion in each of six areas; such discussion as was submitted in writing; a general summary of the Symposium with conclusions drawn by the closing rapporteur; and statements by representatives of the three sponsoring organizations outlining the present and probable future activity of these organizations in furthering the performance concept in buildings. The subject matter covered in the papers includes physiological, anthropometrical, psychological, sociological, and economic human requirements and methods of evaluation; physical requirements and methods of evaluation in mechanical, acoustical, thermal, dimensional stability, compatibility, fire properties, and geometry areas; operation and main-



tenance requirements and methods of evaluation in such areas as maintenance, repair, replacement, and versatility; techniques and problems in applying the performance concept to design; and experience gained in application of the performance concept in design, building, and building use.

**SP362. Chemical kinetics in the C-O-S and H-N-O-S systems: A bibliography—1899 through June 1971**, F. Westley, Nat. Bur. Stand. (U.S.), Spec. Publ. 362, 68 pages (Apr. 1972).

**Key words:** Bibliography; carbon oxysulfides; carbon sulfides; chemical kinetics; gas phase; hydrogen; nitrogen; nitrogen oxides; oxygen; sulfur; sulfur hydrides; sulfur oxides.

A bibliography, a reaction oriented list of references, is provided for published papers and reports containing rate data for reactions of COS, COS<sub>2</sub>, CS, CS<sub>2</sub>, CS<sub>3</sub>, D<sub>2</sub>S, H<sub>2</sub>S, H<sub>2</sub>S<sub>2</sub>, HSO<sub>2</sub>, S, SH, SO, SO<sub>2</sub>, SO<sub>3</sub>, SO<sub>4</sub>, S<sub>2</sub>, S<sub>2</sub>O<sub>2</sub>, S<sub>4</sub>, S<sub>6</sub> and S<sub>8</sub> with each other and with CO, CO<sub>2</sub>, D, D<sub>2</sub>, H, H<sub>2</sub>, H<sub>2</sub>O, N, N<sub>2</sub>, N<sub>2</sub>O, N<sub>2</sub>O<sub>5</sub>, NO, NO<sub>2</sub>, NO<sub>3</sub>, NOS, O, OH, O<sub>2</sub>, O<sub>3</sub>, R and RH. Three lists of critical reviews dealing with the above reactions are included. 317 papers covering 240 reactions are listed. The period covered extends from 1899 through June 1971.

**SP363. Bibliography on atomic energy levels and spectra, July 1968 through June 1971**, L. Hagan and W. C. Martin, Nat. Bur. Stand. (U.S.), Spec. Publ. 363, 103 pages (June 1972).

**Key words:** Atomic energy levels; atomic spectra; bibliography; energy levels, atomic; spectra, atomic; wavelengths, atoms and ions.

The bibliography contains approximately 1100 references classified by subject for individual atoms and atomic ions. A number index identifies the references. An author index is included. References included contain data on energy levels, classified lines, wavelengths, Zeeman effect, Stark effect, hyperfine structure, isotope shift, ionization potentials, or theory which gives results for specific atoms or atomic ions.

**SP364. Solid state chemistry.** Proceedings of the 5th Materials Research Symposium sponsored by the Institute for Materials Research, National Bureau of Standards, Oct. 18-21, 1971, held at Gaithersburg, Md., R. S. Roth and S. J. Schneider, Jr., Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 364, 799 pages (July 1972).

**Key words:** Chalcogenides; crystallographic shear; electron optical lattice images; lone pair geometry; non-stoichiometry; oxides; refractory hard metals; Solid State Chemistry.

This book presents the Proceedings of the 5th Materials Research Symposium on "Solid State Chemistry" held at the National Bureau of Standards, Gaithersburg, Md., on Oct. 18-21, 1971. The symposium was sponsored by the Institute for Materials Research, NBS. The purpose of the conference was to explore the realm of new inorganic crystalline materials emphasizing crystal chemical and structural aspects, providing a forum for discussion of new research problems and techniques. A total of 56 invited and contributed papers were presented. In addition, the symposium included three unscheduled talks and an open discussion period consisting of four impromptu lectures on very current subjects dealing with nonstoichiometry. The Proceedings are divided into four main groupings, I Oxides, II Borides, Carbides, Silicides, and Related Materials, III Chalcogenides, and IV Open Discussion on Nonstoichiometry. An edited version is given of the floor discussion following each paper. *These proceedings include the following papers (indented):*

**The stereochemistry of the inert pair in some solid oxides or oxide fluorides of Sb<sup>3+</sup>, Bi<sup>3+</sup> and Pb<sup>2+</sup>**, S. Andersson and A. Åström, *SP364*, pp. 3-14 (July 1972).

**Key words:** Antimony oxide fluorides; antimony oxides; bismuth oxide fluorides; lead oxides; lone pairs.

Geometrically it is shown that the inert electron pair in some solid oxides or oxide fluorides requires space comparable with that of an anion. If the lone pairs are located on certain sites in a lattice, nets consisting of lone pairs and anions are obtained which correspond to hexagonal, or cubic closest packing of atoms. Other more complex nets, comparable with those in alloy structures, are also found. The lone pairs are thus found in positions which are normally occupied by anions. Using this observation, direct structural relationships with the transition metal compounds can be shown to exist.

**The single crystal x-ray structure determination of some alkali metal molybdates and niobates**, B. M. Gatehouse, D. J. Lloyd, and B. K. Miskin, *SP364*, pp. 15-27 (July 1972).

**Key words:** Alkali metal; bronze; heptagonal holes; hexagonal tungsten bronze; lattice image; molybdate; molybdenum; niobate; niobium; oxide; single crystal; tetramolybdate; x-ray structure determination.

Crystal structures have been determined for the compounds "Rb<sub>3</sub>Nb<sub>5</sub>O<sub>146</sub>," "RbNb<sub>3</sub>O<sub>9</sub>" Na<sub>x</sub>Mo<sub>6</sub>O<sub>17</sub>, K<sub>x</sub>Mo<sub>6</sub>O<sub>17</sub> (x approximately 0.8 and 1.0 respectively) and Li<sub>2</sub>Mo<sub>4</sub>O<sub>13</sub> (low temperature form). Preliminary results are communicated for the compounds Li<sub>x</sub>Mo<sub>6</sub>O<sub>17</sub> (x ≤ 1.0) and Li<sub>2</sub>Mo<sub>4</sub>O<sub>13</sub> (high temperature form).

For "Rb<sub>3</sub>Nb<sub>5</sub>O<sub>146</sub>" an unusual structure occurs where niobium-oxygen octahedra are grouped forming four, five, six and seven-sided tunnels through the structure, with the hexagonal tunnels partly filled with rubidium atoms. The unbalanced electrostatic charge is discussed in terms of the possible presence of fluoride, or fractional occupancy of oxygen sites.

Unusual features are discussed for the M<sub>x</sub>'Mo<sub>6</sub>O<sub>17</sub> structures (M' = Li, Na, K) in terms of the presence or absence of Mo-O<sub>6</sub> octahedra or Mo-O<sub>4</sub> tetrahedra in the structure. It appears that the lithium analogue will have a somewhat different structure in spite of similarity in unit cell dimensions.

The ordering of lithium-oxygen octahedra in planes in Li<sub>2</sub>Mo<sub>4</sub>O<sub>13</sub> is pointed out in an accurate structure determination of this compound, which is basically a cubic close-packed oxygen lattice with Li and Mo occupying octahedral sites. Systematically absent oxygen atoms result in the presence of pairs of strings of cube octahedral holes in the structure.

**The crystal chemistry of some new mixed oxides of tellurium + IV**, J. Galy, *SP364*, pp. 29-39 (July 1972).

**Key words:** Crystal structure; "lone pair" structures; tellurites; tellurium dioxide; tellurium hypovanadate; titanium tellurite.

The structural chemistry of some new mixed oxides between TeO<sub>2</sub> and some transition metal oxides is discussed.

A new structural type MTe<sub>3</sub>O<sub>8</sub> has been found in the TeO<sub>2</sub>-MO<sub>2</sub> systems (M = Ti, Zr, Hf and Sn). The structure of TiTe<sub>3</sub>O<sub>8</sub> determined by x-ray single crystal analysis is cubic, space group Ia3 with a = 10.956 Å. The relationships with the fluorite structure type have been established. ZrTe<sub>3</sub>O<sub>8</sub> as well as fourteen new compounds with the general formula A<sub>1/2</sub>B<sub>1/2</sub>Te<sub>3</sub>O<sub>8</sub> (A = Sc, Cr, Fe, Ga, Rh, In, Bi and B = Nb, Ta) are isostructural with TiTe<sub>3</sub>O<sub>8</sub>.

In the system TeO<sub>2</sub>-VO<sub>2</sub> the phase TeVO<sub>4</sub> has been prepared in two different crystalline forms, which we designate α and β here. A reversible polymorphic transfor-

mation occurs at 650 °C  $\alpha \rightleftharpoons \beta$ . Both phases crystallize in the monoclinic system. The  $\alpha$ -TeVO<sub>4</sub> crystals are black and the  $\beta$ -TeVO<sub>4</sub> crystals green; a melt of TeVO<sub>4</sub> gives a black glass by quenching. In  $\alpha$ -TeVO<sub>4</sub> the coordination number of vanadium and tellurium is 6 and 3, in  $\beta$ -TeVO<sub>4</sub> the C.N. is 5 and 4.

The crystal structure of NaVTeO<sub>5</sub> (KVTeO<sub>5</sub>, RbVTeO<sub>5</sub> and AgVTeO<sub>5</sub> are isostructural) exhibits isolated chains with (VTeO<sub>5</sub>)<sub>n</sub><sup>n-</sup> formula surrounded by sodium atoms.

Finally, relationship between the structure of  $\alpha$ - and  $\beta$ -TeVO<sub>4</sub> and other "lone pair" structures such as  $\alpha$ -Sb<sub>2</sub>O<sub>4</sub> or SbNbO<sub>4</sub>,  $\beta$ -Sb<sub>2</sub>O<sub>4</sub> and Pb<sub>3</sub>O<sub>4</sub> is discussed, and comparison with such simple structures as  $\alpha$ -PbO<sub>2</sub>, ReO<sub>3</sub>, PdF<sub>3</sub> and TiO<sub>2</sub> rutile also made.

**Crystal structure and physical properties of a triclinic sodium tungsten oxide**, H. F. Franzen, H. R. Shanks, and B. H. W. S. deJong, *SP364*, pp. 41-50 (July 1972).

**Key words:** Resistivity; Seebeck coefficient; sodium tungstate; structure.

A triclinic sodium tungstate was prepared by the method of electrolysis of molten mixtures of Na<sub>2</sub>WO<sub>4</sub> and WO<sub>3</sub> which has been used extensively in the preparation of sodium tungsten bronzes. The electrical resistivities and Seebeck coefficients of several samples were measured and are reported. A single crystal x-ray diffraction study yielded the tungsten atom positions. A structure is suggested which is consistent with the tungsten positions and the electrical properties. The suggested stoichiometry is Na<sub>6</sub>W<sub>14</sub>O<sub>45</sub>. In the suggested structure the tungsten atoms are coordinated by distorted octahedra of oxygen atoms in all cases but one, in which case the tungsten is coordinated by a trigonal-bipyramid of oxygen atoms. The octahedra share corners in planes in a fashion similar to that found in the hexagonal bronze, and the sodium atoms are located in the resulting hexagonal holes.

**Electrochemical preparation and characterization of alkali metal tungsten bronzes**, M<sub>x</sub>WO<sub>3</sub>, M. S. Whittingham and R. A. Huggins, *SP364*, pp. 51-62 (July 1972).

**Key words:** Crystal growth; electrolysis; non-stoichiometry; reaction mechanisms; thermodynamics; tungsten bronze.

When a current is passed through two inert electrodes immersed in a molten solution (~750 °C) of alkali metal tungstate, M<sub>2</sub>WO<sub>4</sub>, and tungsten oxide, WO<sub>3</sub>, oxygen is liberated at the anode and a crystal of tungsten bronze, M<sub>x</sub>WO<sub>3</sub>, where 0 < x < 1, formed at the cathode. The potential difference between the electrodes is related to the oxygen concentration gradient across the cell. Thus, if the electrical potential difference across the cell, rather than the current or current density, is kept constant, crystals with a fixed oxygen activity and hence composition (stoichiometry) will be grown. Measurements of the decomposition potential of melts of M<sub>2</sub>WO<sub>4</sub> and WO<sub>3</sub> of different composition, and of the oxygen activity in tungsten bronzes allows a type of phase diagram relating oxygen activity to the alkali metal/tungsten ratio in both liquid and solid phases to be constructed. Using this thermodynamic approach, it is possible to rule out certain suggested reaction intermediates in the electrolytic process and to explain both the overlapping stoichiometric ranges of some phases and the effects of reacting electrodes on the decomposition potential.

**Some aspects of the investigation of intergrowth phases in Nb<sub>2</sub>O<sub>5</sub>-rich systems**, R. Gruhn, *SP364*, pp. 63-86 (July 1972).

**Key words:** Analysis; hybrid phase; intergrowth phase;

niobium pentoxide; preparation; ranges of homogeneity; stability; systems.

Numerous Nb<sub>2</sub>O<sub>5</sub>-rich compounds with complicated compositions could be prepared as monophasic samples. The preparative and analytical work in this field was supplemented by x-ray investigations using the Guinier technique. In addition to 5 phases (Nb<sub>11</sub>O<sub>27</sub>, Nb<sub>25</sub>O<sub>62</sub>, Nb<sub>28</sub>O<sub>70</sub>, Nb<sub>31</sub>O<sub>77</sub>F, Nb<sub>34</sub>O<sub>84</sub>F<sub>2</sub>) whose structures are known from investigations by Wadsley, Andersson, and Norin, we found 4 "hybrid" phases also called intergrowth-phases. The building principle of the hybrid phases NbO<sub>2.464</sub>, NbO<sub>2.483</sub>, Nb(O,F)<sub>2.510</sub>, and Nb(O,F)<sub>2.523</sub> is a combination of building elements of both neighbor phases, e.g., NbO<sub>2.483</sub> combines component rows of the Nb<sub>25</sub>O<sub>62</sub>-structure and the Nb<sub>28</sub>O<sub>70</sub>-structure in a ratio 1:1.

It is of special interest that the phases Nb<sub>25</sub>O<sub>62</sub>, Nb<sub>28</sub>O<sub>70</sub>, Nb<sub>31</sub>O<sub>77</sub>F, and Nb<sub>34</sub>O<sub>84</sub>F<sub>2</sub> have small but exactly reproducible ranges of homogeneity. The fundamental reason for this deviation from the ideal composition is still unknown. It may be that the deviation from the ideal composition is due to the special properties of the building elements. According to this the non-ideal composition of a hybrid phase may be derived from the non-ideal composition of both neighbor phases, e.g., the actual composition NbO<sub>2.483±0.001</sub> of the hybrid phase may be calculated from the actual limits of the phases Nb<sub>25</sub>O<sub>62</sub> (2.478 O/Nb) and Nb<sub>28</sub>O<sub>70</sub> (2.489 O/Nb). A hybrid phase with the ideal composition 2.491 O/Nb (Nb<sub>25</sub>O<sub>62</sub> + Nb<sub>28</sub>O<sub>70</sub>) is nonexistent.

In addition to the combination of compositions of neighbor phases there may be relationship between the stabilities of the basic structures and the resulting hybrid phases.

**The application of electron optical techniques to high temperature materials**, J. G. Allpress, *SP364*, pp. 87-111 (July 1972).

**Key words:** Crystallographic shear planes; crystal structure; electron diffraction; electron microscopy; lattice images; lithium ferrites; lithium lutetium titanate; niobium-titanium oxides; niobium-tungsten oxides; tungsten oxides; Wadsley defects.

Careful studies of phase equilibria in many high temperature systems have revealed unexpectedly complex structural relationships, which are frequently very difficult to unravel by means of conventional x-ray techniques. The purpose of this contribution is to indicate how and why the electron microscope can be used to advantage in these circumstances. The value of the technique will be demonstrated by referring to the following recent applications in the field of the structural chemistry of oxides: (1) The determination of unit cell data for microcrystalline samples of alkali metal rare earth titanates, using electron diffraction. These materials have orthorhombic superlattices of the perovskite structure; (2) The use of dark field microscopy to study the precipitation of the ferrimagnetic spinel LiFe<sub>5</sub>O<sub>8</sub> from a nonstoichiometric matrix of  $\alpha$ -LiFeO<sub>2</sub>. The morphology of the precipitate depends critically upon prior thermal treatment; (3) The direct observation of crystallographic shear planes in WO<sub>3-x</sub> (x < 0.05) and WO<sub>3</sub> · yNb<sub>2</sub>O<sub>5</sub> (y = 0.03-0.09). The results show how changes of composition are accommodated in these systems, and provide clues as to the mode of formation and diffusion of crystallographic shear defects; (4) The study of regions of "solid solution" in the system TiO<sub>2</sub>-Nb<sub>2</sub>O<sub>5</sub> (> 50 mol % Nb<sub>2</sub>O<sub>5</sub>), by lattice imaging. Variations in composition are accommodated by coherent intergrowth, at the unit cell level, of thin slabs of several parent phases; and (5) The study of phases in the



system  $\text{WO}_3\text{-Nb}_2\text{O}_5$  which have structures related to that of tetragonal tungsten bronze. Several different superlattices are possible, and lattice images provide direct evidence for order-disorder, microdomain formation, and intergrowth with material having a much simpler cubic structure.

**Application of infrared and Raman spectroscopy to the characterization of order-disorder in high temperature oxides.** W. B. White and V. G. Keramidas, *SP364*, pp. 113-126 (July 1972).

**Key words:** Corundum structure; order-disorder; Raman spectra; rocksalt structure; rutile structure; spinel structure.

The vibrational spectra of oxides are remarkably sensitive to ordering effects and are a useful characterization tool. Cation ordering can be classified into: (a) preferential distribution of nonequivalent cations onto nonequivalent sites with no change in space group symmetry or unit cell size, (b) preferential distribution onto equivalent sites with decrease in space group symmetry only, (c) building of superstructures with same symmetry as parent structure, (d) both (b) and (c) combined. Experimental Raman spectra of various structures are compared with these schemes. Ordering of type (a) produces only frequency shifts with no change in spectral pattern and is exemplified by normal-inverse ordering in spinels. Ordering of type (b) produces additional bands due to selection rule relaxation and is exemplified by ilmenite,  $\text{LiNbO}_3$ , and  $\text{Ni}_3\text{TeO}_6$  orderings on corundum and by spinels with 1:1 ordering on tetrahedral sites. Ordering of type (c) produces a multiplicity of bands as is illustrated by the trirutile structure. Ordering of type (d) produces very complex spectra. Examples include: P3c1 ordering on corundum, 1:1 ordering on rocksalt and the Ruddlesden-Popper superstructures. Raman spectra are sharp but intensities are highly variable. Simple ordering schemes are easy to discern, but complex schemes produce spectra difficult to interpret.

**A study of  $\text{V}_2\text{O}_3$  by photoelectron spectroscopy.** J. M. Honig, H. E. Weaver, and R. D. Board, *SP364*, p. 127 (July 1972).

**Key words:** Metallic-insulator transition; photoelectron spectroscopy;  $\text{V}_2\text{O}_3$ .

The occupied energy states of single crystal and polycrystalline  $\text{V}_2\text{O}_3$  have been studied by x-ray photoelectron spectroscopy both above and below the metallic-antiferromagnetic insulator (M-AFI) transition. All of the elemental vanadium and oxygen states in the range 20 to 640 eV below the Fermi level were also encountered in  $\text{V}_2\text{O}_3$ . In addition, a valence band with structure was observed in the range 0 to 10 eV. In the metallic phase this band was intersected by the Fermi level; below the transition temperature the topmost portion of the band was no longer observable, and may have disappeared under increased noise. Under the experimental conditions involving a resolution of 0.3 to 0.5 eV, a search was made for the presence of localized states in the energy spectrum of the insulating phase at 77 K. No such states were encountered; unless they were masked by the residual valence band approximately 4 eV in width it must be concluded that the transition does not involve a change from a localized to an itinerant electron regime.

**Observations in the electron microscope of lattice planes and migration of silver in beta alumina.** W. L. Roth, *SP364*, pp. 129-137 (July 1972).

**Key words:** Beta alumina; electron microscope; lattice images; migration of silver; silver whiskers.

Beta alumina is the commonly accepted name for a sodium aluminate of variable composition and structure with

"ideal" formula  $\text{NaAl}_{11}\text{O}_{17}$ . There is considerable interest in beta alumina and its isomorphs because the monovalent ions diffuse rapidly at temperatures of 300 °C and below. Crystal structure and density studies of the sodium and silver isomorphs have shown the compound is nonstoichiometric and contains approximately 25 percent excess sodium or silver. All of the monovalent ions lie in basal planes at  $z = 1/4$  and  $3/4$ . The planes are separated by 11 Å and ion conduction takes place by two dimensional diffusion in these planes.

The conducting planes have been resolved in the electron microscope and their identity established by electron diffraction. High resolution photographs show lattice bending and rotation.

When relatively thick crystals of silver beta alumina are observed in the electron microscope, worm-like filaments or whiskers about 50 Å in diameter exude from the edge of the crystal. The filaments were shown by electron diffraction to be silver. The filaments are produced by diffusion of  $\text{Ag}^+$  ions down channels in the conducting planes to neutralize the negative charge of absorbed electrons.

**Beta alumina—prelude to a revolution in solid state electrochemistry.** M. S. Whittingham and R. A. Huggins, *SP364*, pp. 139-154 (July 1972).

**Key words:** Beta alumina; diffusion; electrochemical cell; electrochemical transducer; ionic conductivity; mass transport; solid electrolyte.

For almost two decades solid state electrochemical techniques have been used to study the thermodynamic and transport properties of a number of materials. However, these studies have been restricted essentially to systems utilizing electrolytes containing mobile silver or copper ions at low temperatures, and oxygen ions at high temperatures.

Transport measurements have been made on single crystals of beta alumina, which has the nominal formula  $\text{MA}_{11}\text{O}_{17}$  where M is usually a monovalent cation, to test its suitability as a solid electrolyte. In this and related structures, the monovalent cation can be extremely mobile. By use of a group of novel nonpolarizing solid electrodes, which are fully reversible to the monovalent cation, it has been possible to study the ionic conductivity of a series of beta aluminas containing alkali metals as well as thallium over a wide temperature range. The electronic conductivity of silver beta alumina has also been determined by use of the Wagner asymmetric polarization technique over wide ranges of temperature and oxygen partial pressure.

The results of these studies clearly indicate that the beta alumina family shows excellent promise for use as solid electrolytes, exhibiting high values of ionic conductivity and a very low electronic transference number. These properties were exhibited over extremely wide ranges of temperature, -150 to +820 °C, and oxygen partial pressure,  $10^{-24}$  to 1 atm. The use of beta alumina opens up many new opportunities in solid state electrochemistry, particularly in the study of materials containing monovalent cations.

**Experimental study on the ionicity in the  $\text{TiO}$  phase. An application of the new method of determining the structure factor by high voltage electron diffraction.** D. Watanabe and O. Terasaki, *SP364*, pp. 155-164 (July 1972).

**Key words:** Critical voltage for the 400 of  $\text{TiO}$ ; critical voltage for the 110 of  $\text{TiO}_2$  (rutile); determination of structure factor by high voltage electron diffraction; disappearing effect of the second order reflection in electron diffraction; ionicity in  $\text{TiO}$  crystal; many-beam dynamical interaction in electron diffraction; structure factors for electrons of  $\text{TiO}$ .

It was reported recently that the second order reflection in electron diffraction vanishes at a certain accelerating voltage  $E_c$ , owing to the many-beam dynamical interaction combined with the relativistic change of electron mass [Watanabe, Uyeda and Kogiso, *Acta Cryst.* **A24**, 249 (1968)]. A measured value of  $E_c$  makes it possible to determine very accurately the Fourier coefficient of the potential for the first order, and thus the corresponding value of the x-ray scattering factor [Watanabe, Uyeda and Fukuhara, *Acta Cryst.* **A24**, 580 (1968), **A25**, 138 (1969)].

In the present study, the method has been applied to the disordered TiO phase. The accelerating voltages  $E_c$ , for which Kikuchi lines of the 400 reflection vanish, have been measured using a 500 kV electron microscope. The measured values are 340, 354, 389 and 425 kV, respectively, for  $\text{TiO}_{0.82}$ ,  $\text{TiO}_{0.96}$ ,  $\text{TiO}_{1.16}$ , and  $\text{TiO}_{1.25}$ . To compare the experimental values with calculation, the values of  $E_c$  have been calculated for  $\text{TiO}_{0.82}$  and  $\text{TiO}_{1.25}$ , using theoretical scattering factors of titanium and oxygen atoms of various atomic states. The calculations have been made for free neutral atoms  $\text{Ti}^0$ ,  $\text{O}^0$ , monovalent ions  $\text{Ti}^{1+}$ ,  $\text{O}^{1-}$  and divalent ions  $\text{Ti}^{2+}$ ,  $\text{O}^{2-}$ . The structure factors of the first order have been determined using the measured values of  $E_c$ .

Comparison of the experimental values of  $E_c$  and the first order structure factors with theoretical ones enables us to discuss the ionicity in a TiO crystal. The result shows that the ionicity depends on the oxygen concentration in the crystal, i.e., titanium and oxygen atoms in the oxygen-deficient TiO crystal are considered to be almost neutral, while the elements in the titanium-deficient crystal appear to be in the ionic states.

The possibility of applying the present method to a  $\text{TiO}_2$  crystal of the rutile type is discussed as well.

**The structure and intergrowth of the polymorphic forms of  $\text{ZrO}_2 \cdot 16\text{Nb}_2\text{O}_5$ ,** N. C. Stephenson, J. P. Beale, and D. C. Craig, *SP364*, pp. 165-182 (July 1972).

**Key words:** Crystal structure; intergrowth; lattice-image; polymorphism; zirconium-niobium oxide.

The compound  $\text{ZrO}_2 \cdot 12\text{Nb}_2\text{O}_5$  has been reported to exist in three polymorphic forms, one of which is isostructural with  $\text{TiNb}_{24}\text{O}_{62}$ .

The crystal structures of the remaining two polymorphs have been determined by examining x-ray data collected from a single crystal of the  $\beta$ -monoclinic form. The unit-cell dimensions are  $a = 39.693$ ,  $b = 3.830$ ,  $c = 35.488$  Å,  $\beta = 116.53^\circ$ . 2948 data were collected using a single crystal diffractometer and  $\text{CuK}\alpha$  radiation.

No assumptions were made about the structural features and the basic subcell unit was deduced from the Patterson function. Modifications of this subcell give rise to the remaining two polymorphs, which contain blocks of  $3 \times 3$ ,  $4 \times 4$ , and  $3 \times 4$  corner sharing octahedra. The  $3 \times 4$  blocks are all at the one level and form sheets running parallel to (100). The  $3 \times 3$  and  $4 \times 4$  blocks form sheets which alternate with those just described. The manner in which the sheets fit together determines which polymorph is formed.

Although the structures were solved using standard x-ray procedures, the solutions were facilitated by using features of electron transmission micrographs. These consisted of a regular array of dots and streaks (plane group  $p2$ ) arranged in lines parallel to  $c$ . The spacial distribution and contrast of these dots and streaks, together with their arrangements at antiphase boundaries and fault areas, impose certain restrictions upon structures that can be derived by modifications of the basic subcell.

In terms of structure, the areas of contrast on transmission micrographs can be identified with the different types of block junctions.

**Superstructure of the orthorhombic  $\text{Nb}_2\text{O}_5 \cdot 6\text{ZrO}_2$  type phase(s) in the  $\text{Nb}_2\text{O}_5\text{-ZrO}_2$  and  $\text{Ta}_2\text{O}_5\text{-ZrO}_2$  systems,** R. S. Roth, J. E. Waring, W. S. Brower, and H. S. Parker, *SP364*, pp. 183-195 (July 1972).

**Key words:** Equilibrium;  $\text{Nb}_2\text{O}_5\text{-ZrO}_2$ ; ordered defects;  $\alpha\text{-PbO}_2$ -type phase(s); single crystals; superstructure;  $\text{Ta}_2\text{O}_5\text{-ZrO}_2$ .

The phase previously described as  $\text{Nb}_2\text{O}_5 \cdot 6\text{ZrO}_2$  has been found to have a composition varying from a  $\text{Nb}_2\text{O}_5\text{:ZrO}_2$  ratio of about 2:9 to 2:15. The solidus temperatures of the intermediate compositions studied seem to follow a smooth curve from 1435 to 1640 °C rather than a stepwise function expected from a series of compounds. The x-ray diffraction powder patterns indicate a series of phases with subcells similar to  $\alpha\text{-PbO}_2$  and orthorhombic symmetry. Superstructure lines indicate that these phases have a multiple  $b$  axis. The composition 2:9 corresponds approximately to a structure with a  $b$ -axis multiplicity of seven. The 2:11 composition appears to have a multiplicity of eight, 2:13 a multiplicity of nine and the last composition 2:15, a multiplicity of ten. The intermediate compositions 1:5, 1:6 and 1:7 show superstructure lines halfway between those of the simpler phases on either side, corresponding to multiplicities of 15, 17 and 19 respectively. These multiplicities and compositions thus appear to belong to a homologous series  $M_{n-1}\text{O}_{2n}$  where  $n$  varies from 14-20. However the phase equilibria data do not rule out the possibility of a homologous series  $M_n\text{O}_{2n+1}$ . Compositions in the  $\text{Ta}_2\text{O}_5\text{-ZrO}_2$  system apparently have the same composition vs multiplicity arrangement, however, their melting points are considerably higher.

Single crystals of these phases, prepared by both direct cooling of a melt and utilization of a barium vanadium oxide eutectic flux, have enabled the multiplicities to be completely verified and are now being used for crystal structure determinations. This stabilization of the high pressure form of  $\text{ZrO}_2$  (the orthorhombic structure type) by means of higher valence cations provides an alternate process to the anion deficient stabilization of the cubic fluorite phase.

**Physical and geometrical principles of crystallographic shear in rutile,** L. A. Bursill, B. G. Hyde, and M. O'Keeffe, *SP364*, pp. 197-204 (July 1972).

**Key words:** Crystallographic shear; rutile; swinging shear planes;  $\text{TiO}_2$ ;  $\text{TiO}_2\text{-Cr}_2\text{O}_3$  system.

Recent studies by electron microscopy and diffraction have elucidated many of the structural patterns of formation of homologous series of oxides derived from the rutile structure by crystallographic shear. In this paper, the physical and geometrical principles underlying the formation of planar defects are considered. It is shown that the only crystallographic shear planes expected in systems derived from rutile are those containing  $\langle 111 \rangle$  as observed, e.g., in  $\text{TiO}_{2-x}$  and  $\text{TiO}_2\text{-Cr}_2\text{O}_3$ . These results enable us to establish likely criteria for the development of homologous series in oxide systems. The kinetic consequences of the existence of disordered shear planes (Wadsley defects) are further examined in the light of these developments.

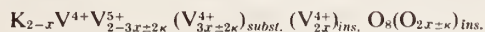
**Structures and chemical bond problems in vanadium oxides,** P. Hagenmuller, *SP364*, pp. 205-218 (July 1972).

**Key words:** Covalence parameters; insulator-metal transitions; perovskite like structures; relations between structures and physical properties; vanadium oxides.



In the transition metal oxides the d-electrons may be either in a localized or a collective state depending essentially on the structure, the transition element and its oxidation state. Some significant examples will be given resulting from recent investigations in the field of the vanadium oxy compounds:

1. A study of the magnetic and electrical properties of the phase  $K_{2-x}V_{3+2x}O_{8+2x+\pi}$   $\phi$  in the system  $V_2O_5$ - $VO_2$ - $K_2O$  shows that it can be written formally as



$K_2V_3O_8$  is actually an insulator in which the  $V^{5+}$  and  $V^{4+}$  ions occupy well defined sites ( $K_2V^{4+}(V^{3+})_2O_8$ ). It does not become a conductor until the progressive appearance of d-electrons in the  $V^{5+}$  sites as a result of a hopping mechanism. The variation with  $x$  of the Curie constant shows that the vanadium, inserted in the form of chain links (O)-V-O-V-(O) in the tunnels emptied by the potassium, also occupies a particular site. These properties were confirmed by the determination of the structure: the phase  $\phi$ , which is isostructural with  $Ba_2TiSi_2O_8$ , is actually made up of three types of cationic sites.

2.  $VO_2$  has an allotropic transformation at 340 K of the type homopolar bonding  $\rightleftharpoons$  metal. This transformation is characterized by a change of symmetry from monoclinic to tetragonal of the rutile type. The replacement of vanadium 4+ by cationic substitution of the type  $2V^{4+}=M^{5+}(Nb^{5+}$  f.e.) +  $V^{3+}$  or by anionic substitution  $V^{4+}+O^{2-}=V^{3+}+F^-$  results in the lowering of the transition temperature. It seems to be the result of the progressive occupancy of a  $\pi$  band. On the other hand the transformation temperature is raised by a substitution of the type  $2V^{4+}=M^{3+}(Cr^{3+}$  f.e.) =  $V^{5+}$ , and there appears an intermediate semi-conducting phase of orthorhombic symmetry. The existence of this phase can be explained by the ferroelectric distortions due to vanadium 5+. The change of the physical properties with the substitution rate is analyzed on the basis of the obtained structures.

3. The phase  $La_{1-x}Sr_xVO_3$  ( $0 \leq x \leq 0.40$ ) with a structure derived from  $GdFeO_3$  is characterized by an evolution from semi-conductor to metal with increasing  $x$ . This latter results from the strengthening of the  $\pi$  (B-O) bond which is a consequence of the weakening of the  $\sigma$  (A-O) bond and the partial replacement of vanadium 3+ by vanadium 4+. This change is less sensitive for the phase  $Gd_{1-x}Sr_xVO_3$ ,  $Gd^{3+}$  being more acidic than  $La^{3+}$  and hence  $\sigma$  (A-O) stronger and  $\pi$  (B-O) weaker.

These results are compared with those obtained for the homologous  $LnTO_3$  phases,  $Ln$  being a lanthanide and  $T$  a 3d-transition element, on the basis of Goodenough's covalent mixing parameters  $\lambda_\pi$  and  $\lambda_\sigma$ . The influence of various factors on the physical properties is discussed.

**Preparation and structure of a pyrochlore and perovskite in the  $BiRhO_{3+x}$  system.** J. M. Longo, P. M. Raccach, J. A. Kafalas, and J. W. Pierce, *SP364*, pp. 219-226 (July 1972).

Key words:  $BiRhO_3$ ; defect structures; perovskite; pressure-synthesis; pyrochlore.

The pyrochlore structure with general formula  $A_2B_2O_7$  is formed with a wide variety of ions and tolerates a high degree of nonstoichiometry on the anion and A cation sites, e.g.,  $Pb_{1.5}Nb_2O_{6.5}$ . We have found that the reaction of  $Bi_2O_3$  with either Rh metal or  $Rh_2O_3$  (Bi/Rh = 1:1) at 600-1000 °C in air or oxygen forms a compound with a face-centered cubic unit cell ( $a = 10.238 \pm .008$  Å) and the pyrochlore structure. X-ray fluorescence for the Bi/Rh ratio and

thermogravimetric analysis for the oxygen content gave  $Bi_{2.0}Rh_{2.0}O_{6.8}$ .

In the pyrochlore structure the cations are in fixed positions, and there are two types of oxygen. Six oxygen atoms are of one type ( $O_1$ ) with one position parameter and form the octahedra around the B cations. The last oxygen ( $O_2$ ) is fixed and coordinated only to the A cations. It is not essential to the  $B_2O_6$ -octahedra network. Taking the origin at the B cation, we have refined the position parameter for  $O_1$ , the occupancy factor (OF) for  $O_2$  and atomic temperature factors (B) by R-factor minimization of integrated powder diffraction intensity data. The results are as follows:

$$B_{Bi} = 0.7, B_{Rh} = 0.1, B_{O_1} = 0.1,$$

$$B_{O_2} = 0.0, x_{O_1} = 0.326, OF_{O_2} = 0.7.$$

The position parameter for  $O_1$  is in agreement with those found in other pyrochlores, and the occupancy factor (OF) is consistent with the chemical analysis. Resistivity measurements on sintered samples at room temperature gave  $\rho = 3.2 \times 10^{-3} \Omega\text{-cm}$ . We will discuss the stability of the defect structure in terms of the availability of the "inert pair" of electrons of the A cation.

When  $Bi_2O_3$  and  $Rh_2O_3$  were reacted in sealed, evacuated quartz tubes at 750-1100 °C, the product could not be identified. When the same reactants were placed in platinum capsules and subjected to over 65 kbar pressure at 1000-1300 °C for 1/2 hour, the perovskite  $BiRhO_3$  was formed. Its unit cell is orthorhombic ( $a = 5.354 \pm .005$  Å,  $b = 5.813 \pm .005$  Å,  $c = 7.776 \pm .005$  Å) as in  $GdFeO_3$  or the series of  $LnRhO_3$ . The relationship between the defect pyrochlore and perovskite structures will be discussed.

**Precious metal pyrochlores.** A. W. Sleight and R. J. Bouchard, *SP364*, pp. 227-232 (July 1972).

Key words: Metallic conductivity; oxides; pyrochlore structure; semiconductivity.

Rare earth pyrochlores of the type  $A_2M_2O_7$  where A is a rare earth and M is Ru, Ir, Pd, or Pt have been reported, but little is known of their physical properties. We have grown crystals of the rare earth ruthenate and iridate pyrochlores. Four-probe electrical resistivity measurements on single crystals show that both rare earth ruthenates and iridates are semiconducting with an activation energy of about 0.1 eV for the ruthenates and about 0.08 eV for the iridates. Very different behavior is found for the iridate and ruthenate pyrochlores when the A cation is a post-transition metal. Although  $Tl_2Ru_2O_7$  is also semiconducting, it has an activation energy of only about 0.01 eV. Metallic conduction is found for  $Tl_2Ir_2O_7$ ,  $Tl_2Os_2O_7$ ,  $Bi_2Ru_2O_7$ , and  $Bi_2Ir_2O_7$ . Magnetic susceptibility measurements confirm the localized electron behavior for the semiconductors and delocalized electron behavior for the metallic compounds. Structural refinements have been carried out for  $Nd_2Ru_2O_7$ ,  $Yb_2Ru_2O_7$ , and  $Bi_2Ru_2O_7$ . The Ru-O distance is  $2.00 \pm .01$  Å for all three compounds; however, an anomalously high temperature coefficient was found for Bi.

**Phases in the systems  $BaO$ - $NiO$ - $O$ - $CO_2$  and  $BaO$ - $CoO$ - $O$ - $CO_2$ .** T. Negas and R. S. Roth, *SP364*, pp. 233-263 (July 1972).

Key words: Ba/Co-oxide phases; Ba/Ni-oxide phases; crystal structure; phase equilibria; transition-metal oxides.

Several new materials apparently related to the aragonite form of  $BaCO_3$  and to the 2H form of " $BaNiO_3$ " were prepared at elevated temperature *in air*. The phases  $Ba_3NiC_xO_{9-y}$  and  $Ba_3Ni_2C_xO_{9-y}$  ( $[Ni+C] \leq 3$ ) were prepared in powder and single crystal form. Both phases are hexagonal with  $a$ -axes related to the 2H " $BaNiO_3$ " by  $a \approx$

$a_{2H}/\sqrt{3}$ . Single crystal x-ray and electron diffraction patterns of the Ba:Ni = 3:1 phase reveal  $c \approx 2c_{2H}$ . The structure was refined in space group P6 to  $R = 5.9\%$  using 639 x-ray reflections. BaCo<sub>3</sub>-3:2 (Ba:Ni) phase composite crystals were prepared by decomposition of 3:1 phase crystals in air at 800 °C. The structure for these composites is discussed. A similar 3:2 compound, Ba<sub>3</sub>Co<sub>2</sub>C<sub>2</sub>O<sub>9-y</sub>, containing low-spin octahedral Co<sup>4+</sup>, was prepared in powder form.

Although 2H "BaNiO<sub>3</sub>" is not stable in air, single crystals of two phases near Ba:Ni = 1:1 were obtained. Both are rhombohedral with hexagonal  $a \approx a_{2H}/\sqrt{3}$  and large c-axis multiplicities but exact stoichiometries are unknown. Two-layer-like forms of BaCoO<sub>3-x</sub> can be prepared in air, however, below 890 °C. Similar phases exist at compositions slightly deficient in cobalt. A 12-layer form of BaCoO<sub>3-x</sub> exists from 890 to 925 °C. It transforms to a phase of unknown structure above 925 °C. The compound Ba<sub>2</sub>CoO<sub>4</sub>, related to Ba<sub>2</sub>TiO<sub>4</sub>, can be prepared above 825 °C. Ba<sub>2</sub>CoO<sub>4</sub> has a reversible, nonquenchable, monoclinic  $\rightleftharpoons$  orthorhombic inversion at 145 °C. The Co<sup>4+</sup> is in a high-spin, tetrahedral, configuration.

**Preparation of SrFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub> and CaFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub> crystals and some of their properties**, E. Banks, O. Berkooz, and T. Nakagawa, *SP364*, pp. 265-273 (July 1972).

**Key words:** Antiferromagnetism; CaFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub>; defect structure; mixed metal oxides; Mössbauer effect; oxygen vacancies; perovskite; semiconductivity; SrFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub>.

Single crystals of SrFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub> and CaFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub> were grown by the usual technique from fluxes of excess SrCl<sub>2</sub> and CaCl<sub>2</sub>, respectively. Apparently cubic perovskites were obtained in the SrFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub> system where x is in the range  $0.4 \leq x \leq 0.7$  and in the CaFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub> where  $x$  is  $0.2 \leq x \leq 0.4$ . Hexagonal crystals, isostructural with the reported high temperature phase of BaMnO<sub>3</sub>, were obtained in the SrFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub> where x is 0.1 and 0. Chemical analysis showed that the values of Fe:Mn ratio in these crystals were very close to the expected ones. From the density and x-ray measurements the existence of substantial amounts of oxygen vacancies ( $0.26 \leq y \leq 0.44$ ) in the perovskite crystals was observed. For the hexagonal crystals, lower concentrations of oxygen vacancies ( $y \sim 0.11$ ) were observed. The Mössbauer spectra of crystals having  $x = 0.4 - 0.7$  in the SrFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub> system were found to consist of two kinds of quadrupole-split lines of Fe<sup>3+</sup> ions, Fe<sup>3+</sup> (I) which are present in regular oxygen octahedra and Fe<sup>3+</sup> (II) which are associated with oxygen vacancies. From the magnetic measurements, Néel temperatures in the SrFe<sub>x</sub>Mn<sub>1-x</sub>O<sub>3-y</sub> were found to be  $T_N = 130, 35$  and  $20$  K for  $x = 0.7, 0.5$  and  $0.4$ , respectively. Using the experimental data of the densities, the Mössbauer effect and effective magnetic moments, discussions concerning the amount of oxygen vacancies in the perovskite compounds are given.

The perovskite-like phases exhibited semiconducting behavior with activation energies of about 0.16 eV, which was almost independent of composition.

**La<sub>2</sub>Sr<sub>1-x</sub>RuO<sub>3</sub>: A new perovskite series**, R. J. Bouchard and J. F. Weiher, *SP364*, pp. 275-284 (July 1972).

**Key words:** Antiferromagnetism; Curie-Weiss paramagnetism; ferromagnetism; metallic conductivity; oxide; perovskite; solid solution.

The compound LaRuO<sub>3</sub> was prepared for the first time. It appears to be metallic and antiferromagnetic. Solid solutions with ferromagnetic SrRuO<sub>3</sub> of the type La<sub>2</sub>Sr<sub>1-x</sub>RuO<sub>3</sub> exist for all values of x. All compounds have the orthorhombic GdFeO<sub>3</sub>-type perovskite structure. The ferromagnetism ob-

served for SrRuO<sub>3</sub> ( $x = 0$ ) diminishes rapidly with increasing La content, and antiferromagnetism or parasitic ferromagnetism sets in at approximately 35% La. All compounds show Curie-Weiss behavior at fairly low temperatures. The properties of LaRhO<sub>3</sub> are also discussed.

**High pressure synthesis and crystal structure of cobalt sesquioxide and its low-spin  $\rightarrow$  high-spin transition**, M. Marezio, P. D. Dernier, J. Chenavas, and J.-C. Joubert, *SP364*, pp. 285-286 (July 1972).

**Key words:** Cobalt sesquioxide; crystal structure; high pressure synthesis; low-spin  $\rightarrow$  high-spin transition.

**Influence of madelung energy and covalency on the structure of A<sup>+</sup>B<sup>3+</sup>O<sub>3</sub> compounds**, J. A. Kafalas, *SP364*, pp. 287-293 (July 1972).

**Key words:** A<sup>+</sup>B<sup>3+</sup>O<sub>3</sub> compounds; ferroelectricity; perovskites; phase stability.

The large Goldschmidt tolerance factor  $t = 1.06$  in BaTiO<sub>3</sub> appears to be related to its ferroelectric properties and also suggests that relatively large effective charge at a Ti<sup>4+</sup> ion inhibits formation of the hexagonal-perovskite polytypes generally associated with  $t > 1.0$ . In order to test these ideas, RbNbO<sub>3</sub> and RbTaO<sub>3</sub> ( $t = 1.08$ ) were prepared under very high pressures. RbNbO<sub>3</sub> is an orthorhombic perovskite isostructural with ferroelectric BaTiO<sub>3</sub>, and it decomposes on heating without formation of an hexagonal-perovskite polytype. Only at 90 kbar and 900 °C did RbTaO<sub>3</sub> form a cubic, or nearly cubic, perovskite. Unlike the transition-metal ions, Sb<sup>5+</sup> and Bi<sup>5+</sup> have never been stabilized in a cubic perovskite structure. AgSbO<sub>3</sub> forms a defect pyrochlore, NaSbO<sub>3</sub> and KSbO<sub>3</sub> have ilmenite structures, although a cubic (Pn3) form of KSbO<sub>3</sub> is stabilized by prolonged annealing above 1000 °C. A body-centered-cubic, disordered form of the cubic KSbO<sub>3</sub> having space group 123 was prepared in five minutes at 20 kbar and 800 °C. Preparation of RbSbO<sub>3</sub> at 20 kbar and 1000 °C yielded a phase with the same structure. These results are interpreted to mean that strong covalent bonding inhibits the formation of 180° Sb<sup>5+</sup>-O<sup>2-</sup>-Sb<sup>5+</sup> linkages.

**Defects in oxides**, J. S. Anderson, *SP364*, pp. 295-317 (July 1972).

**Key words:** Block structures; crystallographic shear; defect clusters; defect models; high resolution electron microscopy; oxide defects; rutile structure; Wadsley defects.

Defects in ionic crystals, such as the metallic oxides, are so intimately involved in diffusion, reactivity and electronic properties, that an understanding of defect structure is a necessary background for a variety of problems in the chemistry, physics and technology of materials. In the present context consideration will be restricted primarily to thermodynamic defects: the inner equilibrium of oxide structures, stoichiometric changes that displace that equilibrium, and solid solutions in which replacement of one cation by another of different valence involves an analogous change in the ratio of cations to anions in the crystal structure. This paper is largely concerned with structural matters and has two purposes: the first is to draw together what is known about highly defective oxide structures (stoichiometrically variable and solid solution phases); the second is to consider, in more detail, one or two systems that exhibit a remarkable capacity for organizing their defect structures.

It has been customary to treat these problems within the framework of point defect theory. This viewpoint, well rooted in statistical thermodynamics, is certainly applicable



to highly ionic uni-univalent crystals (alkali halides) and, perhaps generally to highly dilute defect systems, e.g.,  $10^{19}$  cm<sup>-3</sup> or less. We are concerned with concentrations two orders of magnitude greater, with ions of greater formal charge, and (in the important transition metal oxides) with a considerable measure of orbital overlap between cations and anions and, in some cases, direct cation-cation bonding. These last considerations raise questions about the effects exerted by defects, such as anion vacancies, on charge screening and cation repulsions, and about the preservation of cation coordination so as to maximize charge screening and optimize the covalent component of the bonding.

We shall try to trace a progression in our classification of defect structures, and in doing so we shall find effects both of chemical specificity—the electronic configuration, as well as the size of cations—and of influences exerted non-specifically, by crystal structure type.

**Oxygen dissociation pressures and phase behavior in the transplutonium oxides,** T. D. Chikalla and R. P. Turcotte, *SP364*, pp. 319-330 (July 1972).

**Key words:** Actinide oxides; actinide sesquioxides; americium oxides; berkelium oxides; curium oxides; melting points of actinide oxides; nonstoichiometry; oxides; thermodynamics.

The results of recent oxygen vapor pressure measurements over nonstoichiometric AmO<sub>x</sub>, CmO<sub>x</sub>, and BkO<sub>x</sub> are presented. These include derived information concerning the phase relations and partial thermodynamics of oxygen solution over the range  $1.5 < x < 2.0$  and  $300 < T < 1200^\circ\text{C}$ .

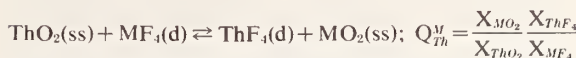
The americium-oxygen system has been examined by thermogravimetric techniques in the single phase  $\alpha$  region for  $1.80 < x < 2.00$  to yield relative partial molar heat and entropy data. Supporting information obtained by quench methods and x-ray diffraction analysis extend the results to lower compositions and, additionally, demonstrate the existence of a bcc  $\sigma$  phase over a wide composition range. Phase relations in the curium-oxygen system have been defined by a series of isobars in the pressure range  $2 < p_{\text{O}_2}$  (mm)  $< 730$ . In addition to  $\alpha$  and  $\sigma$  phase, compounds of more narrow compositional width are seen at CmO<sub>1.72</sub> and CmO<sub>1.82</sub>, and a plausible phase diagram is constructed. Differences obtained on two curium isotopes of greatly different radioactivity are discussed. The berkelium-oxygen system has been examined using a novel capacitance manometer system and a 1.2 mg sample. A set of five isotherms was obtained over the range  $852 < T (^\circ\text{C}) < 1150$ . The isotherms show a regular variation across  $\alpha$  and  $\sigma$  regions separated by a diphasic field at  $x \sim 1.79$ . In addition, a narrow two-phase region exists between BkO<sub>1.91</sub> and BkO<sub>1.93</sub>. Certain similarities are shown to exist between this and certain other fluorite related ternary oxide systems.

In addition, melting behavior of the di- and sesquioxides and polymorphism in the sesquioxide is described over the entire actinide series.

**Binary solid solutions of PaO<sub>2</sub> and other actinide dioxides and their exchange equilibria with molten salt reactor fluorides,** C. E. Bamberger, R. G. Ross, and C. F. Baes, Jr., *SP364*, pp. 331-341 (July 1972).

**Key words:** Activity coefficients in solid solutions; equilibria with molten fluorides; equilibrium of actinide oxides and molten fluorides; heat of mixing in solid solutions; ion exchange between solid oxides and molten fluorides; lattice parameter of actinide oxides; molten fluorides; molten salt reactor; oxide solid solutions; plutonium dioxide; protactinium dioxide; thorium dioxide; uranium dioxide.

The dioxides of thorium, protactinium, uranium and plutonium all are relatively insoluble in molten mixtures—containing LiF, BeF<sub>2</sub>, ThF<sub>4</sub>, PaF<sub>4</sub>, and UF<sub>4</sub> or UF<sub>3</sub>—which serve as the fuel of the molten salt nuclear power reactors (MSR's). Since these dioxides can form substitutional solid solutions, exchange reactions of the type



involving the solid solution (ss) and the molten fluoride phase (d) become possible. It is of interest to study such exchange equilibria not only because the inadvertent precipitation of fissile oxide solids from an MSR fuel should be avoided, but also because such reactions might provide a means of separating and recycling the fissile and fertile elements.

A study of the exchange reaction involving Pa<sup>4+</sup> and Th<sup>4+</sup> has been carried out in which PaO<sub>2</sub>-ThO<sub>2</sub> solid solutions ( $X_{\text{PaO}_2} \leq 0.33$ ) were formed by equilibration of ThO<sub>2</sub> with molten LiF-BeF<sub>2</sub>-ThF<sub>4</sub>-PaF<sub>4</sub> (72-16-12-0.05 mol %) in the temperature range 570-730 °C. The resulting values of the distribution quotient  $Q_{\text{Th}}^{\text{Pa}}$ , along with previously measured values of  $Q_{\text{Th}}^{\text{U}}$  and a value of  $Q_{\text{Th}}^{\text{Pu}}$  derived indirectly from other previous measurements, are consistent with the following expressions

$$\begin{aligned} \ln \gamma_{\text{MO}_2} &= 10^6 \left( \frac{1.228 \pm .15}{T} \right) \left( \frac{\Delta a}{a_{\text{ThO}_2}} \right)^2 X_{\text{ThO}_2}^2; \\ \ln \gamma_{\text{ThO}_2} &= 10^6 \left( \frac{1.228 \pm .15}{T} \right) \left( \frac{\Delta a}{a_{\text{ThO}_2}} \right)^2 X_{\text{MO}_2}^2 \\ \ln Q_{\text{Th}}^{\text{M}} &= 10^6 \left( \frac{1.318 \pm .03}{T} \right) \left( \frac{\Delta a}{a_{\text{MO}_2} a_{\text{ThO}_2}} \right) \\ &\quad + 10^6 \left( \frac{1.228 \pm .15}{T} \right) \left( \frac{\Delta a}{a_{\text{ThO}_2}} \right)^2 (2X_{\text{MO}_2} - 1) \end{aligned}$$

wherein the activity coefficients in the solid solution are related to the difference in the lattice parameters ( $\Delta a = a_{\text{ThO}_2} - a_{\text{MO}_2}$ ) as suggested by Hietala's model.

**Growth and x-ray studies of single crystals of higher oxides of praseodymium and terbium,** M. Z. Lowenstein, L. Kihlberg, K. H. Lau, J. M. Haschke, and L. Eyring, *SP364*, pp. 343-351 (July 1972).

**Key words:** Higher oxides; hydrothermal crystal growth; oxide structures; praseodymium oxide; single crystal; terbium oxide.

Single crystals of higher oxides of praseodymium and terbium have been grown successfully using hydrothermal techniques. Cold seal reactors were utilized to study the crystallization process over a temperature range of 600-900 °C and at pressures up to 3.1 kilobar. Crystal growth conditions were optimized using controlled pressure and temperature cycling. Any oxide of praseodymium may be used as starting material. Nitric acid served both as a mineralizer to promote solubility and as a source of oxygen. Two predominant crystal habits are observed; octahedra and trigonal prisms. Faces are smooth and well defined.

Single crystals of praseodymium dioxide have been reduced to PrO<sub>1.833</sub> in the homologous series Pr<sub>n</sub>O<sub>2n-2</sub> with crystal integrity maintained. X-ray data have been obtained on these crystals using Weissenberg and Hägg-Guinier cameras. The phase has a fluorite-type sublattice with a su-

perstructure of monoclinic symmetry (space group  $P2_1/n, C_2^5h$ ) and a unit cell having  $a = 6.6874 \text{ \AA}$ ,  $b = 11.602 \text{ \AA}$ ,  $c = 15.470 \text{ \AA}$ ,  $\beta = 125.257^\circ$  and  $V = 979.6 \text{ \AA}^3$ . Indexing of the powder pattern of this phase has been completed on the basis of this cell. The relationship to the fluorite subcell is shown.

**Defects and mass transport in reduced  $\text{CeO}_2$  single crystals,** Y. Ban and A. S. Nowick, *SP364*, pp. 353-365 (July 1972).

**Key words:** Ceria; crystal defects; diffusion; mass transport; nonstoichiometry; oxides.

A study is made of reduced  $\text{CeO}_2$  in the form of large single crystals grown by arc fusion. It is shown that, so long as  $y \geq 1.67$  in the formula  $\text{CeO}_y$ , all structural changes on reducing  $\text{CeO}_2$  occur without loss of coherency of the original fluorite lattice. Comparison of length and lattice parameter changes shows that only oxygen vacancies (and no detectable Ce interstitials) are present in the reduced state. For  $y > 1.67$ , it is shown that oxidation (in air or in  $\text{O}_2$ ) takes place at reasonable rates just above room temperature. The kinetics of this anomalously rapid mass transport are studied in some detail, including the effects of sample thickness and of oxygen partial pressure. The results show that the kinetics are neither diffusion nor surface controlled. A model of the process is developed which explains the major results. The low temperature oxidation process does not terminate in the pure  $\alpha$  ( $\text{CeO}_2$ ) phase, but in a metastable structure, here called  $\alpha'$ , for which  $y$  is very close to 2.0. The properties of  $\alpha'$  are discussed.

**Anion centered coordination polyhedra and related physical properties in rare earth oxides and oxysalts,** P. E. Caro, *SP364*, pp. 367-383 (July 1972).

**Key words:** Complex ions; coordination polyhedra; nonstoichiometry; polymolecular frameworks; rare earth optical spectra; rare earth oxide; refractory materials; thin films;  $4f^n$  configurations.

The structures of rare earth oxides and oxysalts can be conveniently described in terms of linkages of anion centered coordination polyhedra, namely tetrahedra, yielding two-dimensional or three-dimensional frameworks. A complex "lanthanyl" cation  $(\text{LnO})_n^{n+}$  can be recognized. It has two different arrangements of tetrahedra, one of them being identical with the well known "bismuthyl" cation  $(\text{BiO})_n^{n+}$ . The structural elements are similar to the classical  $\text{SiO}_2$  and  $\text{Si}_x\text{O}_y$  ones;  $\text{SiO}_4$  tetrahedra frameworks, used for silicates structures classification. Other anions than oxygen (sulfur and halides) yield isomorphous networks.

Such types of structures imply some sort of covalent bonding. The covalence of the bond can be shown from optical measurements on solids. For  $(\text{OLn})_n$  compounds the absorption spectrum is displaced to the red (nephelauxetic effect), a phenomenon which corresponds to the lowering of the Racah's parameters of the  $4f^n$  configuration. The mixing of the  $|4f^n\rangle$  wave functions with ligand wave functions also yields larger transition probabilities and the  $(\text{LnO})_n^{n+}$  materials are very effective phosphors.

The layered oxide structures also yield textured thin films which exhibit epitaxial continuity and intergrowth between the rare earth oxides phases.

The layered polymolecular complex cation concept can be applied to rare earth extended non-stoichiometric systems. It can be shown that the chemical composition of all the known phases of those systems can be accounted for in terms of the succession along a main crystallographic axis of four planar chemical units ABCD. Non-stoichiometry occurs because a layered structure AB is able to be interleaved

through another layered structure ADCD. A general chemical formula for the ordered phases was derived, for the bastnaesite family of compound (AB=bastnaesite, ADCD=synchisite), the  $\text{Ln}_2\text{O}_3\text{-LnF}_3$  systems (AB=tysonite, ADCD=trigonal  $\text{EuOF}$ ), the  $\text{LnO}_x$  systems (AB= $\text{Ln}_6\text{O}_{10}$ , ADCD= $\text{Ln}_{12}\text{O}_{22}$ ) and the  $\text{LnCl}_3\text{-LnCl}_2$  system (AB= $\text{LnCl}_3$ , ADCD= $\text{LnCl}_2$ ). All of the compounds contain layered polymolecular complex cations.

**Plasma-synthesized substoichiometric scandium oxide,** J. E. Young, Jr., and M. J. Sienko, *SP364*, pp. 385-395 (July 1972).

**Key words:** Crystal growth; F centers; flame fusion; magnetic susceptibility; nonstoichiometry; scandium oxide.

Crystals of substoichiometric scandium oxide have been grown in high frequency, induction-coupled, argon plasmas. The composition of the crystals could be varied by addition of small percentages of hydrogen or oxygen to the argon stream. Chemical analysis by reoxidation indicated an oxygen deficiency that could attain 4% before metallic films appeared, concentrated at grain boundaries. The chemical composition of the films could not be established. X-ray studies of the bulk crystals indicated retention of the C-type rare earth structure of  $\text{Sc}_2\text{O}_3$  with but slight shrinkage of the cubic cell parameter. Transmission electron microscopy showed no evidence for shear plane formation. Attempts to measure Hall voltage and conductivity by a van der Pauw technique gave conductivity values, both a.c. and d.c., too small to measure. Faraday susceptibility measurements from 1.6 to 300 K indicated a very small effective magnetic moment, which decreased below 10 K. Possible models are F and F' centers in thermal equilibrium or  $\text{Sc}^{+1}$  ions with thermal equilibrium between  $^3\text{D}$  and  $^1\text{D}$  or  $^3\text{D}$  and  $^1\text{S}$  states.

**Crystal chemistry and compound formation in the systems rare earth sesquioxide- $\text{WO}_3$ ,** G. J. McCarthy, R. D. Fischer, G. G. Johnson, Jr., and C. E. Gooden, *SP364*, pp. 397-411 (July 1972).

**Key words:** Fluorite-related structures; rare earth tungstates; rare earth tungsten oxides;  $\text{RE}_2\text{O}_3\text{-WO}_3$  compounds; RE-W-O systems.

Compounds with the following stoichiometries have been prepared in the rare earth sesquioxide-tungsten trioxide systems:  $\text{RE}_6\text{WO}_{12}$ ,  $\text{RE}_{10}\text{W}_2\text{O}_{21}$ ,  $\text{RE}_{14}\text{W}_4\text{O}_{33}$ ,  $\text{RE}_2\text{WO}_6$ ,  $\text{RE}_2\text{W}_2\text{O}_9$ . Compounds of the first three stoichiometries prepared at  $1400^\circ\text{C}$  have structures apparently related to that of fluorite.  $\text{RE}_6\text{WO}_{12}$  has three structural classes whose symmetries are dependent on the rare earth ionic radius: La-Pr, cubic or pseudocubic; Nd-Gd, pseudotetragonal; Tb-Lu, Y, rhombohedral.  $\text{RE}_{10}\text{W}_2\text{O}_{21}$  is stable only for RE=Gd-Ho, Y and has the same pseudotetragonal symmetry as the intermediate  $\text{RE}_6\text{WO}_{12}$  compounds.  $\text{RE}_{14}\text{W}_4\text{O}_{33}$  has a pseudorhombohedral structure related to the third  $\text{RE}_6\text{WO}_{12}$  structure. The rhombohedral  $\text{RE}_6\text{WO}_{12}$  compounds are known to be isostructural with  $\text{RE}_2\text{O}_3$  oxides and it is suggested that  $\text{RE}_{10}\text{W}_2\text{O}_{21}$  and  $\text{RE}_{14}\text{W}_4\text{O}_{33}$  may be structurally related to  $\text{RE}_4\text{O}_7$  and  $\text{RE}_6\text{O}_{11}$  respectively.  $\text{RE}_2\text{WO}_6$  compounds with RE=Pr-Dy have a monoclinic scheelite-related structure. The  $\text{RE}_2\text{W}_2\text{O}_9$  compounds, also with a complex monoclinic structure, are stable only for RE=Ce-Gd (or Tb). Compounds of the stoichiometries  $\text{RE}_4\text{W}_3\text{O}_{12}$  and  $\text{RE}_2\text{W}_3\text{O}_{12}$  were not studied, but the literature information on them is noted. A discussion of the probable subsolidus phase relations in RE-W-O systems is also included.

**Preparation of oxides and related compounds by chemical transport,** H. Schäfer, *SP364*, pp. 413-436 (July 1972).



**Key words:** Chemical Vapor Transport; crystal growth; oxides; synthesis.

In a temperature gradient it is possible for solids to migrate by sublimation, by catalytic sublimation ( $P_{red}/I_2$ ), dissociative sublimation and by chemical transport.

Reversible heterogeneous reactions are utilized in chemical transport. The phenomenon is complex but can normally be treated as gaseous diffusion between spaces in which thermodynamic equilibrium has been established between solid and gaseous phases. The partial pressure drop between these spaces is the quantity which determines the suitability of a chemical reaction for transport processes.

Information is given regarding working techniques and transport agents which have been employed hitherto.

In further chapters there is an account of the binary oxides which have been chemically transported up to now and there is also an account of the types of reaction used for transport.

Using zinc oxide transport as an example, a demonstration is given of the selection of transport reactions on the basis of thermodynamic considerations.

There is a discussion of syntheses in a temperature gradient and of "solid/solid reactions," with regard to the preparative employment of chemical transport processes. This discussion is illustrated with several examples. There is in addition a review of the transport of ternary compounds and of the decomposition of ternary compounds which can occur under the influence of the transport agent.

Examples are given of the crystallization of metastable modifications out of the gas phase.

**Precision parameters of the ferroelectric rare earth molybdates  $\text{Ln}_2(\text{MoO}_4)_3$ .** L. H. Brixner, P. E. Bierstedt, A. W. Sleight, and M. S. Licit, *SP364*, pp. 437-443 (July 1972).

**Key words:** Ferroelectric molybdates of rare earths; lattice parameters; phase transitions.

Lattice parameters to an accuracy of better than  $\pm 0.001 \text{ \AA}$  have been determined for the ferroelectric  $\text{Ln}_2(\text{MoO}_4)_3$  compounds with  $\text{Ln} = \text{Pr, Nd, Sm, Eu, Gd, Tb, Dy}$  and  $\text{Ho}$ . X-ray patterns were obtained with a Hagg-Guinier camera and the data was refined by a least-squares method using selected reflections. Parameters obtained this way exhibited a systematic trend of the  $b$ - $a$  dimension as a function of the cation size for the orthorhombic  $\text{Pba}2$  room temperature structure. A linear relationship between the cell volume and the cube of the ionic radius of the rare earths has been observed. The first seven compounds are metastable at room temperature and transform from the ferroelectric/ferroelastic  $\text{Pba}2$  structure to the parent  $\text{P4}_2/\text{m}$  structure between 140 and 235 °C. Only  $\text{Ho}_2(\text{MoO}_4)_3$  is stable in the  $\text{Pba}2$  phase at room temperature and transforms into the tetragonal structure at 121 °C. The high temperature structure for this compound is orthorhombic, space group  $\text{Pnca}$ . The transition temperatures have been accurately determined by differential scanning calorimetry, differential thermal analysis, dielectric measurements and hot-stage optical techniques and are discussed in relationship with the degree of  $b$ - $a$  distortion. Lattice parameters have also been determined for the stable monoclinic modification of  $\text{Sm, Eu, Gd, Tb}$  and  $\text{Dy}$ -molybdate and their transition temperatures, ranging from 800 to 1000 °C, as reported.

**Structural and phase relationships among trivalent tungstates and molybdates,** K. Nassau and J. W. Shiever, *SP364*, pp. 445-456 (July 1972).

**Key words:** Crystal structure; lanthanide compounds; molybdates; tungstates.

The trivalent tungstates  $\text{L}_2(\text{WO}_4)_3$ , molybdates  $\text{L}_2(\text{MoO}_4)_3$ , and mixed systems,  $\text{L}_2(\text{W}_{1-x}\text{Mo}_x\text{O}_4)_3$  have been studied between room temperature and the melting points (up to 1650 °C). Single crystal and powder x-ray diffraction at room and elevated temperatures, differential thermal analysis, and crystal growth were among the techniques used to characterize phases and determine relationships.

Among the molybdates of the lanthanides,  $\text{In, Sc, Fe, Cr}$ , and  $\text{Al}$ , at least five structures were observed: the tungstates show at least three. Particular attention was devoted to  $\text{Tb}_2(\text{MoO}_4)_3$ , which, like  $\text{Gd}_2(\text{MoO}_4)_3$ , shows transitions at 800, 1040 and melting at 1155 °C and a ferroelectric transition at 163 °C in the metastable phase region; not all of these transitions are easily reversible.

Pseudo-binary tungstate-molybdate phase diagrams and structural parameters were determined for the  $\text{La, Nd, Sm, Gd, Ho}$ , and  $\text{In}$  systems. Based on structural determinations together with phase diagram interpretations and crystal growth evidence of the nature of various transitions (destructive or nondestructive), structural relationships were used to organize the many structures into three groupings and relate the results to the radii of the trivalent atoms:

(i) The small size tungstates and molybdates, the  $\text{Sc}_2(\text{WO}_4)_3$  type family, with at least two members, form 6-coordinated structures with unit cell or subcell based on  $\text{Pnca}$ ; with rising temperature this family extends to larger size atoms.

(ii) The large size tungstates and molybdates form 8-coordination structures with scheelite related subcells; this  $\alpha\text{-Eu}_2(\text{WO}_4)_3$  type family includes at least 4 structures.

(iii) The  $\beta\text{-Gd}_2(\text{MoO}_4)_3$  type family of structures, occurring only in the intermediate size molybdates, have 7-coordinated trivalent atoms; except for  $\text{Y}_2(\text{MoO}_4)_3$  they are stable only above 800 °C, although extensive metastability does occur with ferroelectric transitions in the metastable form near room temperature.

**Crystal chemistry of tetrahedrally-coordinated oxides:  $\text{Li}_3\text{PO}_4$  derivatives,** A. R. West and F. P. Glasser, *SP364*, pp. 457-469 (July 1972).

**Key words:** Crystal chemistry; kinetics; lithium arsenate; lithium phosphates; lithium vanadate; phase transformation; polymorphism.

The high and low polymorphs of  $\text{Li}_3\text{PO}_4$  are type structures for a large family of tetrahedrally-coordinated oxides. These are readily synthesized by direct solid state reaction of the constituent oxides or by hydrothermal reaction. The simplest substances which are  $\text{Li}_3\text{PO}_4$ -type include  $\text{Li}_3\text{VO}_4$  and  $\text{Li}_3\text{AsO}_4$ , although the high-low inversion in the latter two proceeds reversibly through one or more intermediate phases which are thermodynamically stable over a short range of temperatures.

The intermediate phases often undergo further structural distortion during quenching to ambient.  $\text{Li}_3\text{PO}_4$  itself forms an intermediate phase in the conversion low  $\rightarrow$  high  $\text{Li}_3\text{PO}_4$ . This intermediate phase is readily retained to ambient but is believed to be metastable at all temperatures. More complex  $\text{Li}_3\text{PO}_4$  derivatives include substances of the general formula  $\text{Li}_2\text{MXO}_4$ , where  $\text{M} = \text{Mg, Zn, Co}^{2+}$  and  $\text{X} = \text{Si, Ge}^{4+}$ . Each compound usually has at least two polymorphs. These fall into three classes: one which is either high or low  $\text{Li}_3\text{PO}_4$  type, one which includes the distortional derivatives of both high and low  $\text{Li}_3\text{PO}_4$ , and lastly, phases of related but unknown structures. A full explanation of the polymorphism of an individual phase is only possible if effects due to solid solution are taken into account. For example, the stoichiometry of " $\text{Li}_2\text{ZnSiO}_4$ " varies within the system

$\text{Li}_4\text{SiO}_4\text{-Zn}_2\text{SiO}_4$ ; the solubilities of excess  $\text{Li}^+$  and  $\text{Zn}^{2+}$  have been measured as a function of temperature. Inversion temperatures, and especially, the occurrence and stability of many of the distortional derivative structures, are closely related to the stoichiometry.

The possibilities of making other substitutions, such as replacing  $(\text{Li}^+ + \text{M}^{2+})$  by  $\text{A}^{3+}$ , where  $\text{A} = \text{Al}, \text{Ga}^{3+}$ , etc., are discussed.

This family of phases is probably of widespread occurrence. We have encountered these phases in glass-ceramic systems, such as  $\text{Li}_2\text{O-MgO-ZnO-SiO}_2$ , where they are an important crystallization product of *all* glass composition.

**On the solidification temperature and the nonstoichiometry of cobaltous oxide in an oxidizing atmosphere**, J. P. Coutures and M. Foex, *SP364*, pp. 471-481 (July 1972).

Key words:  $\text{CoO-O}_2$  system; melting point depression; nonstoichiometry in liquid  $\text{CoO}$ ; solar furnace; thermal analysis.

Liquid cobaltous oxide can dissolve a large amount of oxygen depending on temperature oxygen partial pressure and time. Therefore, the solidification temperature decreases when the amount of oxygen in the liquid phases increases. During solidification, a "spitting" phenomena occurs. The behavior (spitting phenomena for example) and the properties of this oxide (solidification temperature, melt composition, solid composition) are studied by high temperature techniques.

**The system  $\text{FeO-SiO}_2\text{-TiO}_2$  at high temperatures and high pressures**, E. Woermann and A. Lamprecht, *SP364*, p. 483 (July 1972).

Key words:  $\text{FeO-SiO}_2\text{-TiO}_2$  system; high pressure; high temperature; ternary system.

The investigations of liquidus and solidus relationships in the system  $\text{FeO-SiO}_2\text{-TiO}_2$  in equilibrium with metallic iron at one atmosphere total pressure revealed four ternary invariant points:

(1)  $\text{L} = \text{wüstite} + \text{fayalite} + \text{ulvöspinel}$  ( $1169^\circ \text{C}$ ); (2)  $\text{L} = \text{fayalite} + \text{tridymite} + \text{ulvöspinel}$  ( $1145^\circ \text{C}$ ); (3)  $\text{L} + \text{ilmenite} = \text{tridymite} + \text{ulvöspinel}$  ( $1180^\circ \text{C}$ ); and (4)  $\text{L} + \text{ferropseudobrookite} = \text{tridymite} + \text{ilmenite}$  ( $1254^\circ \text{C}$ ).

In the system ferropseudobrookite-tridymite-rutile in equilibrium with metallic iron considerable amounts of trivalent titanium are observed at solidus and liquidus temperatures. The titanium bearing phases thus are located outside of the ternary system  $\text{FeO-SiO}_2\text{-TiO}_2$  toward the oxygen deficient side.

At elevated pressures the following reactions occur:

(1)  $\text{Ferropseudobrookite} = \text{rutile} + \text{ilmenite}$ ; (2)  $\text{ulvöspinel} + \text{quartz} = \text{fayalite} + \text{ilmenite}$ ; (3)  $\text{fayalite} + \text{quartz} = \text{ferrosilite}$ ; and (4)  $\text{ulvöspinel} = \text{wüstite} + \text{ilmenite}$ .

Depending on temperature and pressure the iron titanium phases form limited solid solutions in the system  $\text{FeO-SiO}_2$ , due to the occurrence of defect structures.

**Carbides and silicides**, H. Nowotny, H. Boller, and G. Zwillling, *SP364*, pp. 487-504 (July 1972).

Key words: Carbides; chemical bonding; defect structures; interstitial compounds; ordering; silicides.

A brief survey of the structural chemistry of transition element carbides will be presented with emphasis on the problem of carbon-void ordering. The scandium carbides including  $\text{Sc}_{15}\text{C}_{19}$  are to be discussed. Complex carbides which derive from octahedral and trigonal prismatic building

elements will be classified. Metal-metal carbides such as  $\text{VCr}_2\text{C}_2$  and metal-nonmetal carbides such as  $\text{Ti}_3\text{SiC}_2$ ,  $\text{V}_4\text{P}_2\text{C}$ ,  $\text{Nb}_2\text{SC}$  or  $\text{Ta}_2\text{S}_2\text{C}$  will be interrelated. The role of nitrogen and hydrogen on the stabilization of complex carbides such as  $\text{Cr}_3$  ( $\text{C}, \text{N}$ )<sub>2</sub> or  $\text{Zr}_2\text{CH}_{0.5}$  will also be treated. Besides the class of typical interstitial carbides, some examples of metal boro-carbides displaying a two-dimensional boron-carbon network will be given ( $\text{YB}_2\text{C}$ ). In compounds such as  $\text{Cr}_2(\text{P}, \text{C})$  carbon plays an intermediate role. The present state of the problem of chemical bonding in carbides will be discussed.

Binary metal silicides are numerous and occur almost at any composition. They are commonly classified as valence compounds (electronegative), metal-like silicides (electropositive) and clathrate silicides (mainly electroneutral). Disilicides and related compounds exhibit a particularly wide occurrence. The continuous change of structural elements and properties of this group will be discussed. So-called defect disilicides of formula  $\text{T}_n\text{Si}_{2n-m}$  ( $\text{T}$  = transition element) which are derived from the  $\text{TiSi}_2$  type structure belong to a uniform building principle, where  $n$  presents the number of subcells and  $m$  the deviation from the disilicide composition. In many cases a relation of the electronic concentration with  $m$  can be observed. In general, lowering of the overall electron concentration diminishes the defect  $m$ . Single crystal work on  $\text{Mn}_{27}\text{Si}_{47}$  will be described. This phase, a fifth variety having a composition in the vicinity of  $\text{MnSi}_{-1.7}$ , presents the problem of pseudo-homogenous domains. Some ternary silicides such as  $\text{E}$ -phases will be discussed from the viewpoint of ordered structures.

**Investigations in the ternary system—boron-carbon-silicon**, E. Gugel, R. Kieffer, G. Leimer, and P. Ettmayer, *SP364*, pp. 505-513 (July 1972).

Key words: Binary system; boron; carbon; chemical analysis; melting-point determination; metallography; phase-field division; silicon; solubilities; ternary system; x-ray investigations.

Viewing the literature one will notice that the available knowledge about the nonmetallic inorganic systems are rather insufficient and sometimes do not agree with each other. These systems yield a number of attractive high temperature materials and therefore it is essential to improve available information.

The Institut für chemische Technologie anorganischer Stoffe (Institute for Chemical Technology of Inorganic Materials), Technical University of Vienna, and the Research Institute of the Cremer-Group, Rödental-Germany, have systematically worked in this area for several years. This paper will deal with the system Boron-Carbon-Silicon.

In contradiction, some publications confirmed the existence of  $\text{B}_4\text{C}$  only in the enclosing system Boron-Carbon. However, Boron Carbide is able to incorporate excess Boron up to the composition  $\text{B}_{6.5}$  (in solid solution) clearly showing a lattice expansion. Within the enclosing system Silicon-Boron there are the chemical compounds  $\text{SiB}_{4-x}$  ( $x \leq 1$ ) and  $\text{SiB}_{12+x}$  ( $x \geq 8$ ). According to our investigations the ternary system itself, in contrast to some other scientists, does not contain ternary phases as well as no solid solution between enclosing binary systems. Limited solid solutions exist around  $\text{B}_4\text{C}$  (+ Si) and around  $\text{SiB}_{4-x}$  (+ C). The x-ray investigations permit the presentation of phase distributions. By means of a new method for determination the melting temperatures of high temperature materials the liquidus areas (melting isotherms) of this system were investigated.



**Valence bonding in some refractory transition metal compounds with high coordination**, F. L. Carter, *SP364*, pp. 515-559 (July 1972).

**Key words:** Aluminum diboride—cadmium diiodide structure; bidirectional orbitals; effective charge; ESCA; Fermi surface distortion; Madelung constant; Madelung potential; metallic single bond radii; refractory transition metal compounds; tungsten carbide; valence bonding; Voronoi polyhedra.

Bond formation in transition metal compounds isomorphous with WC and  $AlB_2$  is formulated using the bidirectional orbital approximation (BOA) to establish orbital hybridization and a simple but self-consistent application of Pauling's metallic radii with charge transfer to obtain the bond orders. For tungsten carbide seven mutually orthogonal bidirectional bonding orbitals for the negative W atom permit it to simultaneously bond its fourteen neighbors with up to 6.5 electrons. However, bond polarization results in an effective negative charge for carbon of 0.0 to  $-0.3e$ . For the diborides the metallic radii results indicate that the group IV diborides have a slightly positive boron which becomes negative with increasing group number but remains below a charge of  $-1e$ . Four arguments are given for the pleating of the boron layer were it to be heavily charged as has been proposed earlier in the isoelectronic analogy to graphite. One of these involves a new definition of atomic volume based on the Voronoi polyhedron. Bond formation by the boron and carbon atoms in these compounds is discussed using the nonpaired spin-orbital [NPSO] approach of Linnett.

Madelung constant and Madelung potentials calculations via the method of Bertaut have been made for both the tungsten carbide and the  $AlB_2(CdI_2)$  structure. These were computed in order to both estimate the magnitude of the electrostatic stability as a function of atomic parameters and to provide a basis for the comparison of ESCA chemical shift data with the calculated effective charge.

The effect of bond formation in distorting the surfaces of constant energy in  $k$  space is also considered in these compounds with the aid of a simple square well potential model. The principle directions of these distortions of the unreduced Fermi surface are indicated for the WC structures and as a function of the boron position parameter for the  $AlB_2$  structures.

Finally, we note that in both of these structures almost all the electrons outside the rare gas cores are involved in bond formation; this is in contrast to the refractory chalcogenides.

**Crystal chemistry of refractory carbides**, A. L. Bowman, *SP364*, pp. 561-566 (July 1972).

**Key words:** Carbide; crystal structure; molybdenum carbide; niobium carbide; reaction mechanism; solid state; tantalum carbide; tungsten carbide; vanadium carbide.

The crystal structures of most of the refractory metal carbides may be described generally on the basis of a close-packed metal sublattice, with the carbon atoms occupying all or part of the octahedral sites. Close-packed carbide structures have been observed with composition MC and packing type c,  $M_4C_3$  and hhcc,  $M_3C_2$  and hcc or hhc, and  $M_2C$  and h or c. All of these structures have one octahedral site per metal atom, and thus an apparent possible composition MC. This is reached however, only with the c-type packing, and it has been suggested that only one half of the sites adjacent to an h layer can be filled. This is found to be an upper limit that is not always reached. These carbide structures thus have carbon vacancy concentrations ranging from  $\sim 0$  up to  $\sim 70\%$ , with a possibility of vacancy order-

ing. Neutron and electron diffraction studies have shown ordering to exist in the  $M_2C$  compounds and in carbon-deficient VC.

The order-disorder transformation of the carbon vacancies in  $Mo_2C$  has been studied in detail with high-temperature neutron diffraction. The kinetics data are consistent with a nucleation-growth mechanism involving nucleation on grain boundaries and linear growth across the interface. The reaction between  $Mo_2C$  and  $Mo_3C_2$ , involving the transformation of the close-packed metal lattice ( $h \rightleftharpoons hcc$ ) has been studied less thoroughly, but the kinetics data also appear to be consistent with a nucleation-growth mechanism.

**A simple model for the stability of transition metal carbides**, R. G. Lye, *SP364*, pp. 567-582 (July 1972).

**Key words:** Bonding; carbides; cohesive energy; density of states; electronic structure; heat of formation;  $L_{II,III}$  spectra; refractory hardmetals; Ti; TiC; transition metal compounds.

The origins of the unusual and complex combination of physical properties exhibited by the transition metal carbides remain somewhat obscure despite extensive studies of the problem in recent years. Even the qualitative nature of the bonding has not yet been described in a manner that accounts satisfactorily for the diverse and sometimes apparently contradictory experimental observations made on these compounds.

One theme, however, recurring through the years of study, draws attention to the similarity of these compounds to the parent transition metals. This characteristic of the carbides is considered briefly in the present study in an attempt to provide a qualitative explanation for the manner in which the stability of the carbide phases varies with the position of the parent metal in the periodic chart of the elements. A simple model for the d band bonding in the transition metals, discussed by Cyrot-Lackmann, is modified for this purpose. In particular, it is assumed that a major component of the bonding in the carbides arises from crystalline electronic energy bands derived for the d states of the metal atoms. Because of changes in crystal structure, these bands are modified somewhat from the shape of the corresponding bands in the parent metal. Of greater importance for the stability of the carbides, however, is the increase in the width of the band, discussed by Costa and Conte, that results from the presence of the carbon atoms within the interstitial positions in the metal sublattice.

As for the parent metals, the cohesion of the carbides is determined by the number of electrons in the d band. In the carbides, however, it is assumed that some of these electrons are provided by transfer from the 2p states of the carbon atoms. Thus, the stability, as measured by the heat of formation, results from the combined effects of the increase in the width of the d band and in the number of electrons it contains.

Despite the considerable simplifications employed, an analytical formulation of this model yields estimates for the heats of formation of the carbides that agree remarkably well with the experimental data presently available.

**Ordering effects in NbC and TaC**, J. D. Venables and M. H. Meyerhoff, *SP364*, pp. 583-590 (July 1972).

**Key words:** Carbides; electron diffraction; interpretation of ordering effects; niobium carbide; ordering effects; superlattice; tantalum carbide; transition metal compounds; vanadium carbide.

Studies of the phase equilibria in the MC transition metal carbides have shown that they retain their nominal NaCl structure over a relatively wide phase field. Although it is

well known that this wide latitude in composition is accomplished through the incorporation of carbon vacancies in the carbon sublattice, there is considerable uncertainty regarding the degree of order exhibited in most of the carbides by the remaining carbon atoms. In this investigation, an attempt has been made to resolve this question for NbC and TaC using some of the techniques applied previously in a study of ordering in the vanadium-carbon system.

By means of transmission electron microscopy and electron diffraction, evidence has been obtained for the existence of long range carbon atom ordering in single-crystal niobium carbide that has a carbon-to-metal ratio close to the integral composition Nb<sub>6</sub>C<sub>5</sub>. The ordering, which gives rise to superlattice and domain structures similar to those observed in V<sub>6</sub>C<sub>5</sub>, appears, however, only in samples that have been cooled slowly (~8 °C/h) through the order-disorder temperature of 1025 °C. In TaC of similar composition, the ordering, although present, remains very imperfect even after the crystals are subjected to the same thermal treatment.

The results are interpreted in terms of the electronic structure of the transition metal carbides as it is currently understood, and their relevance to the mechanical properties of NbC and TaC are discussed.

**The CdP<sub>2</sub>-Ge system and the growth of crystals of CdGeP<sub>2</sub>, E. Buehler and J. H. Wernick, *SP364*, pp. 591-595 (July 1972).**

**Key words:** CdGeP<sub>2</sub>; CdP<sub>2</sub>-Ge system; Ge; phase diagram; single crystals.

The macroscopic features of the phase relationships in the CdP<sub>2</sub>-Ge system have been determined. The tetragonal CdGeP<sub>2</sub> phase melts congruently at 790 ± 5 °C. Two eutectics are present: one between CdP<sub>2</sub> and CdGeP<sub>2</sub> at ~700 °C and 20 mol % Ge, and the other, between CdGeP<sub>2</sub> and Ge at ~750 °C and 65 mol % Ge. Techniques and results for the growth of crystals from stoichiometric melts, by chemical transport, and from liquid Cd and Sn are presented.

**High boron content rare-earth borides, K. E. Spear and G. I. Solovyev, *SP364*, pp. 597-604 (July 1972).**

**Key words:** Borides; lattice constants; LnB<sub>66</sub> compounds; melting temperatures; microhardness; rare-earth borides.

Investigations were performed to determine which rare-earth metals form LnB<sub>66</sub> phases, and to measure some of the properties of these compounds. Similar rare-earth borides have been recently reported with B:Ln ratios of 50 to 100 for metals Y, Gd, Tb, Ho, and Yb. A single crystal structure analysis published on the yttrium compound shows the structure to be face-centered cubic with an ideal stoichiometry YB<sub>66</sub>. In the present studies, ten representative metals were used: Y, La, Ce, Pr, Nd, Sm, Gd, Dy, Er, and Yb. Boron-rich compositions were prepared by arc-melting mixtures of the elements. Identification of the phases in each sample was performed with the use of x-ray and metallographic techniques. All of the investigated systems except La, Ce, and Pr formed the LnB<sub>66</sub> phase, and it is predicted that all rare-earth metals from Nd through Lu will form this phase. Lattice parameters were measured and show a general, but not regular decrease with atomic number. The LnB<sub>66</sub> phases are extremely hard, with Vickers microhardness values ranging from about 3600 to 4000 kp/mm<sup>2</sup>. Melting temperatures for the LnB<sub>66</sub> phases were essentially the same for all metals, and equal to approximately 2150 °C.

**Preparation and characterization of boron suboxide, D. R. Petrak, R. Ruh, and B. F. Goosey, *SP364*, pp. 605-611 (July 1972).**

**Key words:** Amorphous boron; anhydrous boric acid; boric oxide; boron carbide structure type; boron suboxide; crystal structure; decompose; electron microbeam probe; infrared spectrum; lattice parameters; pycnometer; reaction-hot pressing; rhombohedral boron; x-ray diffraction.

Fabrication techniques have been developed to produce specimens of near theoretical density by reaction hot pressing of boron and boric acid in vacuum at temperatures of 1900-2000 °C and pressures of 0.41 kbars. The composition range 80 to 89 atomic % boron was investigated by chemical analysis, lattice parameter studies, pycnometric density determinations, electron probe analysis and infrared analysis. Results support the B<sub>12</sub>O<sub>2</sub> chemical formula and the R3m space group with twelve boron atoms in the 18h positions and two oxygen atoms in the 6c positions. Thus, on the basis of the experimentally determined hexagonal lattice parameters of  $a = 5.386 \pm 0.003$  Å and  $c = 12.326 \pm 0.004$  Å, the calculated density is 2.602 g · cm<sup>-3</sup> and this is in good agreement with the experimentally determined value of 2.600 ± 0.007 g · cm<sup>-3</sup>. The occupancy of the 3b position by either boron or oxygen (to allow the B<sub>4</sub>O or B<sub>13</sub>O<sub>2</sub> stoichiometry) is ruled out since this would require increases in density and/or lattice parameters and none were observed. Also these configurations do not satisfy the Longuet-Higgins and Roberts counting rule. The boron suboxide phase has been studied by electron probe and infrared analyses. The oxygen K emission spectra as well as the infrared reflection spectra are presented. Boron suboxide has been studied by mass spectrometric analysis and found to decompose to rhombohedral boron and B<sub>2</sub>O<sub>2</sub>.

**Ternary transition metal silicides and germanides: Ordering and metal-metal bonding in Ni<sub>2</sub>In-related phases, V. Johnson and W. Jeitschko, *SP364*, pp. 613-622 (July 1972).**

**Key words:** Fe<sub>2</sub>P and Mn<sub>5</sub>Si<sub>3</sub>; metal-metal bonding; metal-site occupancies; Ni<sub>2</sub>In; ordered ternary silicides and germanides; silicides and germanides; ternary Ni<sub>2</sub>In-related phases; TiNiSi.

Ternary transition metal silicides and germanides with structures related to Ni<sub>2</sub>In ("filled" NiAs) are reviewed. For compositions TT'Si and TT'Ge, where T is a transition metal from groups IV, V and VII and T' is from the iron group, the structures adopted are TiNiSi (ordered anti-PbCl<sub>2</sub>), ordered Fe<sub>2</sub>P, TiFeSi or Ni<sub>2</sub>In. We describe and illustrate how these as well as the hexagonal Mn<sub>5</sub>Si<sub>3</sub> structure are related.

Metal site occupancies in ternary TiNiSi and Fe<sub>2</sub>P-type silicides and germanides and pseudobinaries with Ni<sub>2</sub>In and Mn<sub>5</sub>Si<sub>3</sub> structures are also reviewed. We discuss the importance of the relative size and electronegativity of the transition metal atoms and their d-electron configurations in determining site preferences.

Bonding in these Ni<sub>2</sub>In-related phases, (TT')<sub>2-x</sub>Si(Ge), is discussed. The structures differ principally in the strengths of the respective T-T, T-T', and T'-T' metal-metal interactions. Questions as to how these are determined by electronegativities, size and d-electron configuration, and how they in turn affect phase stability and metal-site occupancies are raised.

**Structural transitions of some transition-metal chalcogenides, F. Jellinek, *SP364*, pp. 625-635 (July 1972).**

**Key words:** Dichalcogenides; intercalation compounds; layer structures; modulated structures; occupation waves; selenides; semiconductor-to-metal transitions; structure transitions; sulfides; tellurides; transition-metal chalcogenides; trigonal-prismatic coordination.



A survey is given of some recent investigations on transition-metal chalcogenides (sulfides, selenides, tellurides) carried out in the author's laboratory; particular attention is paid to compounds undergoing structural transitions at elevated temperatures. Examples are given of transitions involving a change of the coordination of the metal ( $\text{NbSe}_2$ ,  $\text{TaSe}_2$ ,  $\text{MoTe}_2$ ,  $\text{Ni}_3\text{Se}_2$ ), of order-disorder transitions ( $\text{AgCrSe}_2$  and related compounds; chromium sulfides,  $\text{Ni}_{1-x}\text{Te}_2$ ), and of transitions involving distortions of the structure ( $\text{CrS}$ ,  $\text{VS}$ ,  $\text{Nb}_{1-x}\text{S}$ ). The occurrence of trigonal-prismatic coordination in several transition-metal chalcogenides is ascribed to d-covalency which stabilizes trigonal-prismatic with respect to octahedral coordination for ions with a  $d^0$ ,  $d^1$  or spin-paired  $d^2$  configuration. The effect of the metal coordination on the physical properties of the compound is also described. The distributions of occupied and vacant metal sites in transition-metal chalcogenides  $\text{M}_{1+p}\text{X}_2$  are discussed (chromium sulfides, zirconium selenides), as is the concept of "occupation waves" (titanium sulfides). In  $\text{Ni}_{1-x}\text{Te}_2$  occupation waves lead to a phase lacking three-dimensional periodicity; the intervention of this phase allows smooth transitions from the disordered high-temperature form to the ordered low-temperature forms (two-step second-order transition).

**Solid solubility in the face centered cubic  $\text{Gd}_x\text{Se}_{1-x}$  system**, F. Holtzberg, D. C. Cronmeyer, T. R. McGuire, and S. von Molnar, *SP364*, pp. 637-644 (July 1972).

**Key words:** Color-concentration dependence; gadolinium monoselenide; Hall effect; homogeneity range; magnetic ordering; reflectivity; resistivity; single crystal growth.

The range of homogeneity has been studied in the face centered cubic  $\text{Gd}_x\text{Se}_{1-x}$  system. The solid solution field is bounded by the composition  $x = 0.443$  for excess Se and extends through the stoichiometric composition to at least 0.512 for excess Gd. The lattice constant decreases linearly with decreasing Gd concentration except at lowest values of  $x$ . The materials have been characterized by resistivity, reflectivity and magnetic measurements. The results of the transport and reflectivity measurements are explained on the basis of a simple single rigid band model. Magnetization measurements show that all compositions order antiferromagnetically with the Néel temperature,  $T_N$ , varying from  $\sim 20$  to  $\sim 60$  K and  $\theta$  from  $-25$  to  $-135$  K with increasing Gd or electron concentration.

**Ternary chalcogenides of light rare earth elements with transition elements**, G. Collin, H. D. Nguyen, O. Gorochoy, M. Guittard, P. Laruelle, and J. Flahaut, *SP364*, pp. 645-650 (July 1972).

**Key words:** Crystal structure; magnetic properties; rare earth; ternary chalcogenides; transition metals.

Description of three new crystal families. Crystal structures. Magnetic properties. (1)  $\text{La}_2\text{Fe}_2\text{S}_5$ -type — orthorhombic  $\text{A2}_1\text{am}$ ; (2)  $\text{La}_8\text{Fe}_3\text{S}_{15}$ -type — monoclinic  $\text{Bm}$ . These two structures have similarities. The rare earth atoms are 7-8 coordinated. The Fe atoms have two kinds of environments: 4-coordinated in a distorted tetrahedron of S atoms, 6-coordinated in a distorted octahedron of S atoms. In both cases 2 neighboring Fe atoms are associated by 2 intermediate S atoms. These 4 atoms form a distorted quadrilateral with Fe-S-Fe angles not far from  $90^\circ$ ; (3)  $\text{CeCrSe}_3$ -type — orthorhombic  $\text{Pnam}$ . The rare earth atoms are 9-coordinated, and the Cr atoms are 6-coordinated, inside a nearly regular octahedron of selenium. As in the preceding structures, 2 neighboring Cr atoms form with 2 intermediate S atoms a nearly regular square.

These compounds are antiferromagnetic at low temperature (Néel temperature for  $\text{LaCrSe}_3$ : 165 K). Weak ferromagnetism appears at lower temperature.

**Crystal chemistry of metal-rich refractory sulfides**, H. Chen and H. F. Franzen, *SP364*, pp. 651-662 (July 1972).

**Key words:** Crystal structure; intermetallic; phosphides; refractory; sulfides; transition metal; coordination polyhedra.

Systematization of the crystal structures of metal-rich chalcogenides was attempted with emphasis on the coordinations of a few key metal atoms. This approach gave a more complete interpretation of many chalcogenide structures, notably those of  $\text{Ta}_2\text{S}$ ,  $\text{Ta}_6\text{S}$  and  $\text{Nb}_2\text{Se}$ , than did the conventional descriptions using the packing of the coordinations of the chalcogen atoms. The pursuit of this approach led to the recognition of a polyhedron, which, owing to its repeated presence in many metal-rich compounds, appeared to be of great importance in crystal chemistry. It is a two-centered polyhedron formed by the interpenetration of two C. N. 14 Kasper polyhedra in such a way that the center of one of the Kasper polyhedra is the apex of another. The presence of a very short interatomic distance between the two centers is one of the important features of this polyhedron. With the help of this polyhedron as the building block, the structures of  $\text{Zr}_9\text{S}_2$ ,  $\alpha\text{-V}_3\text{S}$  and  $\beta\text{-V}_3\text{S}$  were satisfactorily described and correlated; the short interatomic distances in the structures could be explained semi-quantitatively; and the structural differences expressed by the different packing schemes of the polyhedra and the different positions the sulfur atoms occupied in the polyhedra. The description using the two-centered polyhedra as the basic units was extended to the structures in phosphide systems and provided new structural evidences to the similarities and distinctions among the  $\text{Zr}_9\text{S}_2$ -,  $\alpha\text{-V}_3\text{S}$ -,  $\beta\text{-V}_3\text{S}$ -,  $\text{Fe}_3\text{P}$ - and  $\text{Ti}_3\text{P}$ -type structures, and to the correlation that the  $\text{Fe}_3\text{P}$  structure is the high temperature form of the  $\text{Ti}_3\text{P}$  structure. The smooth correlation between the sulfides,  $\text{Zr}_9\text{S}_2$ ,  $\alpha\text{-V}_3\text{S}$  and  $\beta\text{-V}_3\text{S}$ , and the phosphides and related compounds renders further support to the speculation that these sulfides possess the nature of intermetallic compounds.

**Mixed cation disulfides of titanium, vanadium, and chromium**, L. E. Conroy and K. R. Pisharody, *SP364*, pp. 663-671 (July 1972).

**Key words:** Disulfides; electrical conductivity; magnetic properties; sulfides; titanium disulfide; titanium-vanadium disulfides; vanadium disulfide.

Mixed cation disulfides of the types  $\text{Ti}_{1-x}\text{V}_x\text{S}_2$  and  $\text{Ti}_{1-x}\text{Cr}_x\text{S}_2$  have been prepared with compositions in the range  $0 < x < 1$  in the Ti-V system and  $0 < x < 0.4$  in the Ti-Cr system. Polycrystalline materials were prepared by direct reaction of the elements in vacuo at  $950^\circ$ . Single crystals of the Ti-V compounds were prepared by chemical transport reactions, employing iodine as the transport agent. The Ti-Cr disulfides failed to transport by this technique. The chemical properties of the mixed cation materials were found to be very similar to those of  $\text{TiS}_2$ . X-ray diffraction data indicated a random substitution of V or Cr for Ti in the normal Ti sites in the  $\text{TiS}_2$  structure. A regular variation of lattice parameter with the vanadium content was observed in the Ti-V system. The magnetic properties of both the Ti-V and Ti-Cr compounds were characteristic of ferrimagnetic materials, with magnetic susceptibilities in the range of  $3 \times 10^{-11} \text{ m}^3/\text{g}$  to  $12 \times 10^{-11} \text{ m}^3/\text{g}$  (corrected) at room temperature. All of the mixed cation materials exhibited metallic

electrical conductivity in contrast with the degenerate semiconductor behavior of  $\text{TiS}_2$ , with resistivities of the order of  $10^{-5}$  ohm-m at room temperature. No superconductivity was observed at temperatures above 1.3 K. A band model for the description of the electronic properties of these materials is discussed.

**Crystal growth and properties of some I-III-VI<sub>2</sub> compounds,** H. M. Kasper, *SP364*, pp. 671-679 (July 1972).

**Key words:**  $\text{AgGaS}_2$ ; chalcogenides; chalcopyrite; I-III-VI<sub>2</sub> compounds; crystal growth;  $\text{CuGaS}_2$ ;  $\text{CuInS}_2$ ; d-bands; direct bandgap semiconductors; nonlinear optical materials; semiconductor materials.

The I-III-VI<sub>2</sub> compounds are ternary analogues to the II-VI semiconductors and are interesting both as possible nonlinear optical materials and as semiconductors. They usually crystallize in the chalcopyrite structure which belongs to the uniaxial acentric crystal class 42m. In order to study their optical and semiconductor properties, single crystals of  $\text{AgGaS}_2$ ,  $\text{CuGaS}_2$  and  $\text{CuInS}_2$  have been grown by slowly cooling melts of stoichiometric composition, and the conditions of growth by directional freezing are reported.  $\text{AgGaS}_2$  crystallizes as yellow and green crystals. The yellow crystals seem to be gallium rich.  $\text{CuGaS}_2$  does not melt congruently. Stoichiometric melts first crystallize a composition near  $\text{Cu}_{0.88}\text{Ga}_{1.04}\text{S}_2$  as light orange crystals. Later darker, nearly stoichiometric crystals are obtained.  $\text{CuInS}_2$  crystallizes between 1050 and 1000 °C with all crystals transparent to beyond 10  $\mu$ . There is a strong absorption in  $\text{CuGaS}_2$  near 1.8  $\mu$ , which extends toward the visible and causes the darker color. The bandgaps are 2.72 eV for  $\text{AgGaS}_2$ , 2.53 eV for  $\text{CuGaS}_2$  and 1.55 eV for  $\text{CuInS}_2$  at 2 K. Both the light and dark crystals of  $\text{CuGaS}_2$  as well as  $\text{CuInS}_2$  and  $\text{AgCuS}_2$  show sharp line luminescence. The linear and nonlinear optical properties of  $\text{AgGaS}_2$ ,  $\text{Cu}_{0.88}\text{Ga}_{1.04}\text{S}_2$  and  $\text{CuInS}_2$  have been investigated. Unfortunately in both  $\text{Cu}_{0.88}\text{Ga}_{1.04}\text{S}_2$  and  $\text{CuInS}_2$  the birefringence is not large enough to permit three frequency phase matching, but  $\text{AgGaS}_2$  can be phase matched in the infrared for both parametric oscillation and second harmonic generation. With both  $\text{CuGaS}_2$  and  $\text{CuInS}_2$  a pronounced structure has been observed in electrorreflectance near the bandgap and at higher energies. From this structure is concluded that the crystal field splitting of the d bands is about 0.7 eV and that the d bands lie about 2 eV below the valence band edge in both compounds. Stimulated emission has been observed in  $\text{AgGaS}_2$ ,  $\text{CuGaS}_2$  and  $\text{CuInS}_2$ .  $\text{AgGaS}_2$  is usually of high resistivity, whereas  $\text{CuGaS}_2$  is p-type and  $\text{CuInS}_2$  can be made both p- and n-type.

**Crystal chemistry and magnetic properties of phases in the Ba-Fe-S(Se) systems,** H. Steinfink, H. Hong, and I. Grey, *SP364*, pp. 681-694 (July 1972).

**Key words:** Crystal structures of  $\text{Ba}_2\text{FeS}_3$ ,  $\text{Ba}_2\text{FeSe}_3$ ,  $\text{BaFe}_2\text{S}_3$ ,  $\text{BaFe}_2\text{Se}_3$ ,  $\text{Ba}_7\text{Fe}_6\text{S}_{14}$ ,  $\text{Ba}_7\text{Fe}_6\text{S}_{15}$ ,  $\text{Ba}_3\text{Fe}_3\text{Se}_7$ ; magnetic characteristics of  $\text{Ba}_2\text{FeS}_3$ ,  $\text{Ba}_7\text{Fe}_6\text{S}_{14}$  and  $\text{Ba}_6\text{FeS}_{15}$ .

The crystal structures of a number of new phases synthesized in the Ba-Fe-S and Se systems were investigated by x-ray diffraction techniques.  $\text{Ba}_2\text{FeS}_3$  is orthorhombic, Pnma,  $a = 12.087(5)$  Å,  $b = 4.246(2)$  Å,  $c = 12.359(5)$  Å,  $\rho_{\text{meas}} = 4.0$  g/cc,  $\rho_{\text{calc}} = 4.47$  g/cc,  $Z = 4$ , m.p.  $> 1300$  °C. The compound is isostructural with  $\text{Ba}_2\text{ZnS}_3$  and the structure consists of  $\text{FeS}_4$  tetrahedra sharing corners to form an infinite linear chain.  $\text{Ba}_2\text{FeSe}_3$  is isostructural with the sulfide and its parameters are  $a = 12.350(7)$  Å,  $b = 4.439(2)$  Å,  $c = 12.921(5)$  Å.  $\text{BaFe}_2\text{S}_3$  is orthorhombic, Cmc,  $a = 8.7835(9)$  Å,  $b = 11.219(1)$  Å,  $c = 5.2860(5)$  Å,  $\rho_{\text{meas}} = 4.0$

g/cc,  $\rho_{\text{calc}} = 4.40$  g/cc,  $Z = 4$ , m.p.  $= 765 \pm 10$  °C. Three dimensional x-ray diffraction data was used to refine the structure which consists of two  $\text{FeS}_4$  tetrahedra sharing edges and this binuclear unit in turn shares edges with others to form an infinite chain. The structure of  $\text{BaFe}_2\text{Se}_3$  is essentially the same as that of the sulfide but they are not isostructural. The selenide is orthorhombic, Pnma,  $a = 11.878(3)$  Å,  $b = 5.447(2)$  Å,  $c = 9.160(2)$  Å,  $\rho_{\text{calc}} = 5.44$  g/cc,  $Z = 4$ ; decomposes above 750 °C.  $\text{Ba}_7\text{Fe}_6\text{S}_{15}$  is tetragonal, I4/m,  $a = 11.408(2)$  Å,  $c = 10.256(2)$  Å,  $\rho_{\text{meas}} = 4.30$  g/cc,  $\rho_{\text{calc}} = 4.36$  g/cc,  $Z = 2$ , m.p.  $880 \pm 10$  °C. The structure was determined from three dimensional x-ray diffraction data and consists of a tetranuclear unit formed by 4  $\text{FeS}_4$  tetrahedra sharing corners and these units then share edges to form an infinite column.  $\text{Ba}_3\text{Fe}_3\text{Se}_7$  is hexagonal,  $P6_3mc$ ,  $a = 10.843(3)$  Å,  $c = 7.384(2)$  Å,  $\rho_{\text{calc}} = 5.00$  g/cc,  $Z = 2$ . The structure was determined using three dimensional single crystal x-ray diffraction data and consists of isolated trinuclear units formed by edge sharing of three  $\text{FeS}_4$  tetrahedra. The Fe-Fe distances between chains are 6 Å, and vary from 2.6 Å to 4.2 Å within the chains. The Fe-S distances are 2.3–2.4 Å, the S-Fe-S angles are tetrahedral and the Ba-S distances are essentially equal to the sum of the ionic radii. The corresponding distances in the selenides reflect the larger size of the anion.

The magnetic characteristics of  $\text{Ba}_2\text{FeS}_3$ ,  $\text{Ba}_7\text{Fe}_6\text{S}_{14}$  and  $\text{Ba}_6\text{FeS}_{15}$  were investigated; all three compounds are antiferromagnets. The values of the exchange forces, J/k, correlate with the observed Fe-Fe distances.

**Study of sulfospinels,** R. E. Tressler and V. S. Stubican, *SP364*, pp. 695-702 (July 1972).

**Key words:** Flash evaporation; high pressure phases; sulfospinels; thin films.

Several new compounds with the formula  $\text{AB}_2\text{S}_4$  were synthesized. Pressure-induced polymorphism of the sulfospinels was investigated. Sulfospinels which produced new high-pressure phases were  $\text{NiRh}_2\text{S}_4$ ,  $\text{FeYb}_2\text{S}_4$ ,  $\text{In}_2\text{S}_3$ ,  $\text{CrIn}_2\text{S}_4$ ,  $\text{NiIn}_2\text{S}_4$ ,  $\text{CoIn}_2\text{S}_4$  and  $\text{MnIn}_2\text{S}_4$ . The only sulfospinels which transformed to the NiAs derivatives were those in which A and B atoms had unfilled d-orbitals. P-T phase relations were investigated for a series of sulfochromites.

Thin films of several  $\text{ACr}_2\text{S}_4$  (A = Mn, Fe, Co, Cu and Zn) sulfospinels were prepared by a flash evaporation technique on the (111) and (100) planes of NaCl and on the (100) plane of MgO.

**Phase changes in  $\text{Cu}_2\text{S}$  as a function of temperature,** W. R. Cook, Jr., *SP364*, pp. 703-712 (July 1972).

**Key words:** Chalcocite;  $\text{Cu}_2\text{S}$ ; digenite; djurleite; non-stoichiometry; phase relations.

The high-copper phase boundary of  $\text{Cu}_2\text{S}$  deviates from stoichiometry above 300 °C, first becoming copper deficient, then above  $\sim 1075$  °C becoming copper rich. The maximum copper content occurs at the monotectic temperature of 1104 °C. The strong effect of oxygen on the hexagonal-cubic transition in  $\text{Cu}_2\text{S}$  was confirmed; the transition was also found to be sensitive to the type of pretreatment of the material. The high temperature tetragonal " $\text{Cu}_{1.96}\text{S}$ " phase is stable between  $\text{Cu}_{1.95}\text{S}$  and  $\text{Cu}_2\text{S}$ , at temperatures of  $\sim 90$  to  $\sim 140$  °C. The transition to the tetragonal phase is extremely sluggish. The true composition of djurleite has been shown to be approximately  $\text{Cu}_{1.93}\text{S}$ .

The phases near the chalcocite-digenite region of the diagram may be grouped into those with hexagonal close



packing of sulfur atoms and those with cubic close packing of sulfurs. This is important in understanding rates of transformation among the various phases that occur in this area of the diagram.

**Preparation and properties of the systems  $\text{CuFeS}_{2-x}$  and  $\text{Cu}_{1-x}\text{Fe}_{1+x}\text{S}_{2-y}$ ,** R. L. Adams, P. Russo, R. J. Arnott, and A. Wold, *SP 364*, pp. 713-719 (July 1972).

**Key words:** Chalcopyrite;  $\text{CuFeS}_2$ ;  $\text{CuFeS}_{2-x}$ ;  $\text{Cu}_{1-x}\text{Fe}_{1+x}\text{S}_{2-y}$ ; Cu-Fe-S system;  $\text{CuFeS}_2$  crystal growth.

Stoichiometric samples of  $\text{CuFeS}_2$  were prepared by direct combination of the elements in sealed evacuated silica tubes. The products were characterized by x-ray diffraction, density determination, magnetic susceptibility and Mössbauer spectroscopy. Homogeneous single phase products gave a density of  $4.18 \pm 1$  g/cc and cell parameters of  $a_0 = 5.292 \pm (5)$  Å and  $c_0 = 10.407 \pm (5)$  Å. In addition, all of the iron was found to be trivalent and located on tetrahedral sites. The plot of inverse susceptibility versus temperature was nearly temperature independent from 77 to 300 K, and the magnetic susceptibility measurements gave a  $\chi_M = 9.8 \times 10^{-4}$  emu/mole. Single crystals of  $\text{CuFeS}_2$  were grown from the melt by means of a modified Bridgman technique.

Samples having the composition  $\text{CuFeS}_{2-x}$  were also prepared by the direct combination of the elements. X-ray diffraction studies indicated that existence of a single phase, tetragonal  $\gamma$ -form, when  $x$  was varied from 0.17 to 0.24. The compound  $\text{CuFeS}_{1.8}$  had cell dimensions of  $a_0 = 10.598 \pm (5)$  Å and  $c_0 = 5.380 \pm (5)$  Å. Contrary to previous reports, this phase was found to be stable from room temperature to 800 °C. In addition, this phase was stable at room temperature for a period of time in excess of 250 days. It was concluded from density measurements that the structure is best represented as a close packing of sulfur with excess metal ions occupying additional lattice sites.

Compounds having the composition  $\text{Cu}_{1-x}\text{Fe}_{1+x}\text{S}_{1.80}(0.25 > x > 0.08)$  were prepared and found to be cubic with an average cell size of  $a_0 = 5.32$  Å. However, attempts to prepare single phase products with a composition of  $\text{Cu}_{1+x}\text{Fe}_{1-x}\text{S}_{2-y}$  were unsuccessful.

**Laser Raman spectra of polycrystalline  $\text{ZnS}$  and  $\text{Zn}_x\text{Cd}_{1-x}\text{S}$  solid solutions,** J. Shamir and S. Larach, *SP364*, p. 721 (July 1972).

**Key words:** Laser Raman spectra; polycrystalline;  $\text{ZnS}$ ;  $\text{Zn}_x\text{Cd}_{1-x}\text{S}$ .

Raman spectra of polycrystalline  $\text{ZnS}$  and of  $\text{CdS}$  have been recorded. The instrument consisted mainly of a He-Ne laser, Spectra-Physics, model 125 and a 1400 Spex double monochromator. The lines observed were in good agreement with those observed before in a single crystal. Some of these lines are not as sharp and intense as in a single crystal; however, the LO frequency of  $\text{ZnS}$  at  $351 \text{ cm}^{-1}$  is a very sharp and intense line.

In addition we studied the spectra of  $\text{Zn}_x\text{Cd}_{1-x}\text{S}$  solid solutions. These materials have been prepared by firing mixtures of pure  $\text{ZnS}$  and  $\text{CdS}$ , in the proper compositions, at  $1100^\circ\text{C}$ , in an atmosphere of purified Argon. It has been observed that the LO frequency of  $\text{CdS}$  at  $306 \text{ cm}^{-1}$  shifts toward higher frequencies as the concentration of zinc increases. This behavior indicates a type I change as discussed by Pershan and Lacina, namely a linear shift of the frequency as the concentration varies from zero to one in the  $\text{Zn}_x\text{Cd}_{1-x}\text{S}$ . These results resemble the ones obtained in a Vegard plot of lattice constants as determined by x-rays.

**Novel method for the synthesis of rare earth chalcogenides,** C. Paparoditis and R. Suryanarayanan, *SP364*, p. 723 (July 1972).

**Key words:** Coevaporation of elements; rare earth chalcogenides; synthesis.

A description is given of an all-metal vacuum system for the synthesis of rare earth tellurides and selenides by the coevaporation of the elements. The evaporation chamber is provided with three crucibles so that ternary compounds can also be prepared. Forty or more deposits can be obtained in a single operation. A wide range of compositions can thus be obtained if desired. The substrates, amorphous or crystalline, can be heated up to  $600^\circ\text{C}$ . The following compounds have been obtained as polycrystalline, highly textured or single crystal films:  $\text{EuTe}$ ,  $\text{EuSe}$ ,  $\text{YbTe}$ ,  $\text{YbSe}$ ,  $\text{YbSe}_{1.6}$ ,  $\text{SmTe}$ ,  $\text{SmSe}$ ,  $\text{SmSe}_{1.6}$  ( $\text{Th}_3\text{P}_4$  structure),  $\text{Eu}_{1-x}\text{Pb}_x\text{Te}$ ,  $\text{Eu}_{1-x}\text{Gd}_x\text{Se}$ ,  $\text{Eu}_{1-x}\text{Yb}_x\text{Te}$ . Evidence of high quality is given by x-ray, electron microscopy, electron diffraction and electron microprobe analysis. Optical absorption spectra up to 6 eV, reflection spectra up to 10 eV, magnetic circular dichroism spectra in the visible have been obtained. Transition assignments have been proposed for the first time in the case of Yb and Sm monochalcogenides.

Results of optical and magneto optical investigations have been presented for the ferromagnetic  $\text{EuS}$  obtained by coevaporation and for  $\text{EuO}$  obtained by reactive evaporation. Finally, electrical and other transport properties of stoichiometric  $\text{EuO}$  have also been presented.

**SP365. Metric conversion card,** J. V. Odom, *Nat. Bur. Stand. (U.S.)*, Spec. Publ. 355, 2 pages (Revised Nov. 1972).

**Key words:** Metric units, conversion customary to metric; metric units, conversion metric to customary.

A pocket card for convenient appropriate conversion of the customary units of physical measurement to metric units and metric units to customary units.

**SP366. Bibliography on atomic line shapes and shifts (1889 through March 1972),** J. R. Fuhr, W. L. Wiese, and L. J. Roszman, *Nat. Bur. Stand. (U.S.)*, Spec. Publ. 366, 165 pages (Sept. 1972).

**Key words:** Atomic; instrumental broadening; line shapes; line shifts; pressure broadening; resonance broadening; Stark broadening; Van der Waals broadening.

This is the first general, annotated bibliography on atomic line shapes and shifts. It covers exhaustively the atomic spectral line broadening literature in about 1400 separate references extending from 1889 through March 1972. The bibliography contains four major parts: (1) All general interest papers are catalogued according to the broadening mechanisms (and, further, according to special topics under several of the mechanisms), and as to whether the work is a general theory, a general review, a table of profiles or parameters, a comment on existing work, a study of general experimental measurement techniques, or an experimental effort of general importance. Also included are selected papers on important applications of line broadening and on miscellaneous topics relating to atomic spectral line shapes and shifts. (2) In Part 2, all papers containing numerical data are ordered as to element, ionization stage, broadening mechanism (in the case of foreign gas broadening the perturbing species are listed), and it is indicated whether the data are experimentally or theoretically derived. (3) While in the two preceding parts of the bibliography the references are listed for brevity by identification numbers only, in Part 3 all references are listed completely by journal, authors, and title and are arranged chronologically and alphabetically within each year according to the principal

authors. (4) A final section contains a list of all authors and their papers.

**SP367. National Bureau of Standards Brochure, 1972, W. E. Small, Editor, Nat. Bur. Stand. (U.S.), SP367, 66 pages (Dec. 1972).**

**Key words:** National Bureau of Standards; organization; overview; program descriptions.

This publication presents an in-depth look at the National Bureau of Standards. An overview of the Bureau's history, programs, and major contributions precedes individual chapters detailing the programs of each of the four NBS Institutes: Institute for Basic Standards; Institute for Materials Research; Institute for Applied Technology; and Institute for Computer Sciences and Technology. Supersedes NBS Miscellaneous Publication 282 and Special Publication 360.

**SP368. Electrical engineering units and constants, G. F. Montgomery, Nat. Bur. Stand. (U.S.), Spec. Publ. 368, 2 pages (1972).**

**Key words:** Constants; definitions; electricity; electronics; engineering; metric; symbols; units.

This pocket reference card lists a selection of the units and constants used in electrical and electronics engineering. Standard symbols are given for quantities, units, physical constants, and the decimal prefixes used in the International Metric System (SI). Rounded values of the selected physical constants are included.

**SP372. Laser induced damage in optical materials: 1972. Proceedings of a Symposium Sponsored by the American Society for Testing and Materials and by the National Bureau of Standards, June 14-15, 1972, NBS, Boulder, Colo., A. J. Glass and A. H. Guenther, Editors, Nat. Bur. Stand. (U.S.), Spec. Publ. 372, 215 pages (Oct. 1972).**

**Key words:** IR windows and mirrors; laser damage; laser materials; self-focusing; thin films.

The fourth ASTM Symposium on Laser Induced Damage in Optical Materials was held at the National Bureau of Standards in Boulder, Colo., on June 14-15, 1972. This symposium is held as part of the activity of Subcommittee II on Lasers and Laser Materials, of the ASTM. Subcommittee II is charged with the responsibility of formulating standards for laser materials, components, and devices. The chairman of Subcommittee II is Haynes Lee of Owen-Illinois, Inc. Co-chairmen for the damage symposia are Dr. Arthur H. Guenther of the Air Force Weapons Laboratory, and Professor Alexander J. Glass, Chairman of the Department of Electrical Engineering at Wayne State University.

Approximately 125 attendees at the symposium heard 21 papers on topics relating to laser induced damage in glass, crystalline materials, nonlinear optical materials, thin film dielectric coatings, and infrared components. Particular attention was given to the process of plasma formation at dielectric surfaces, the role played by self-focusing in bulk damage in solids, damage morphology of thin film coatings, and the role of absorption in IR component failure.

The proceedings of these Symposia represent the major source of information in the field of laser induced damage in optical materials. The Symposia themselves, along with the periodic meetings of Subcommittee II, provide a unique forum for the exchange of information regarding laser materials specifications among the manufacturers and users of laser devices, components, and systems. The Symposium also serves as a mechanism of information gathering, to enable the Subcommit-

tee to write informed and realistic specifications. *These proceedings include the following papers (indented):*

**Laser damage of HOYA Laser Glass, LCG-11, T. Izumitani, K. Hosaka, and C. Yamanaka, SP372, pp. 3-10 (Oct. 1972).**

**Key words:** HF treatment; inclusion damage; passive and active testing; platinum inclusion; surface damage; thin film coating.

In HOYA Glass Works we have developed a Barium Crown Laser Glass, LCG-11. It has a stimulated emission cross section ( $\sigma$ ) of  $2.0 \times 10^{-20} \text{ cm}^2$  and a loss coefficient ( $\gamma$ ) of  $0.001 \text{ cm}^{-1}$ .

In this report we show that, while platinum lowers the damage threshold of laser glass, by controlling the number and size of the platinum inclusion, the damage threshold of platinum crucible melts of LCG-11 laser glass does not go below  $400 \text{ J/cm}^2$  in the passive test, nor below  $28 \text{ J/cm}^2$  in the active test. This compares favorably with the damage threshold of melts in  $\text{SiO}_2$  and ceramic crucibles. The ceramic melted glass showed a higher lasing threshold, a lower slope efficiency in normal oscillation and an output saturation tendency in Q-switched oscillation.

We find that surface damage is independent of glass strength, glass thermal expansion, and adsorption of water in glass surface. We find that LCG-11 glass, upon treatment with hydrofluoric acid, was improved from  $28 \text{ J/cm}^2$  to  $40 \text{ J/cm}^2$ , a higher damage threshold in passive test, yet we were unable to find a change in glass surface composition due to hydrofluoric acid treatment by using electron microprobe. We assume that surface damage is dependent upon the multi-photon ionization tendency of a glass surface. This assumption is based upon our observation of silica glass which has no single-bond oxygen and a high damage threshold.

**Interaction gradients, concurrent light scattering experiments and bulk laser damage in solids, C. Y. She and D. F. Edwards, SP372, pp. 11-14 (Oct. 1972).**

**Key words:** Bulk; crystalline quartz; fused quartz; interaction gradient; laser glass; laser induced damage; light scattering; stimulated Brillouin scattering.

The concept of interaction gradient and its role on bulk laser damage is discussed. Results of light scattering experiments concurrent with damaging laser pulses on crystalline quartz, fused quartz and laser glass samples are compared to substantiate the role of interaction gradient and stimulated Brillouin scattering on bulk laser damage in solids.

**Optical index damage in electrooptic crystals, A. M. Glass, G. E. Peterson, and T. J. Negran, SP372, pp. 15-26 (Oct. 1972).**

**Key words:** Holographic measurements; laser induced index change; optical memories; reversible low power damage.

Optically induced refractive index changes which occur at low incident power densities ( $< 1 \text{ KW/cm}^2$ ) in many electrooptic crystals have severely limited the application of these materials in the visible spectrum. Following a brief historical review of the subject, we discuss the recent advances in the understanding of the physical mechanisms involved, progress in reducing the damage susceptibility, and in enhancing the effect for holographic applications.

Particular attention is paid to  $\text{LiNbO}_3$  and  $\text{LiTaO}_3$  crystals. Optical and EPR studies of these materials have demonstrated that  $\text{Fe}^{2+}$  impurity ions present in nominally pure material are responsible for the index damage. The ef-



fects of stoichiometry variation, heat treatment, impurity and color center content, X-irradiation of crystals and the kinetics of the index damage process are accounted for by  $\text{Fe}^{2+}$ - $\text{Fe}^{3+}$  reactions.

By careful control of crystal growth and stabilization of the  $\text{Fe}^{3+}$  impurity ion state,  $\text{LiNbO}_3$  and  $\text{LiTaO}_3$  crystals with greatly improved damage resistance have been prepared.

**Comparison of laser induced bulk damage in alkali-halides at 10.6, 1.06, and 0.69 microns**, D. W. Fradin, E. Yablonovitch, and M. Bass, *SP372*, pp. 27-39 (Oct. 1972).

Key words: Alkali halides; avalanche breakdown; bulk damage; self-focusing; surface damage.

It has long been recognized that catastrophic self-focusing cannot occur below a critical power  $P_c$  and that perturbations from self-focusing become progressively less important as the power of a probe optical beam is lowered below  $P_c$ . Using this fact, we have designed and conducted a number of experiments to study bulk damage in alkali-halides in which self-focusing was eliminated and unequivocal measurements of damaging fields obtained. Strongly focusing optical systems were used so that damage could be achieved while probe powers could be restricted to between one and two orders-of-magnitude below theoretical critical powers for electrostrictive self-focusing. Experimental evidence confirms the absence of self-focusing.

By observing the absolute magnitude of breakdown strengths and relative values among the alkali-halides, striking similarities between 10.6, 1.06, and 0.69  $\mu\text{m}$  and d.c. avalanche breakdown were found. The results also showed no frequency dispersion over the wavelength range of 10.6 to 0.69 microns. The implications of this work for surface damage studies are explored and, in addition, the effects of inclusions on bulk optical strength are considered.

**Laser induced damage to glass surfaces**, N. L. Boling and G. Dube', *SP372*, pp. 40-45 (Oct. 1972).

Key words: Chemically strengthened glass; glass damage; glass lasers; laser damage; Q-switched; surface damage.

Entrance and exit surface damage thresholds for Owens-Illinois ED-2 laser glass are measured at Brewster's angle and near normal incidence. A theory that accounts for the observed asymmetry in exit/entrance face damage thresholds is presented. The nature of the damage at both surfaces is described for both untreated and chemically strengthened ED-2 laser glass.

**The relation between surface damage and surface plasma formation**, C. R. Giuliano, *SP372*, pp. 46-54 (Oct. 1972).

Key words: Entrance and exit surface damage; sapphire; spatial and temporal plasma resolution; streak camera experiments; surface plasmas.

A number of experiments are described in which entrance and exit surface laser-induced damage on sapphire samples are studied. Damage thresholds are measured as a function of beam size and divergence at the surfaces. Temporal evolution of surface plasmas is studied using a streaking camera, and spatial differentiation of surface plasmas is accomplished by allowing the light to strike the surfaces away from normal incidence. It is found that the entrance surface has two plasma components, an air plasma which is directed along the light beam and an "explosion" plasma which is directed normal to the surface. The exit surface has only the explosion plasma. It is concluded that surface plasmas are a result of rather than a cause of surface damage.

**Ion beam polishing as a means of increasing surface damage thresholds in sapphire**, C. R. Giuliano, *SP372*, pp. 55-57 (Oct. 1972).

Key words: Ion beam polishing; sapphire; surface damage; threshold increase; threshold measurement.

Polishing of sapphire surfaces with energetic  $\text{Ar}^+$  ion beams is shown to result in a substantial increase in laser damage threshold over that for conventionally polished surfaces. Data for both entrance and exit damage are presented. The results are interpreted in terms of an increase in surface strength with ion beam polishing.

**Laser-induced damage probability at 1.06 and 0.69  $\mu\text{m}$** , M. Bass and H. H. Barrett, *SP372*, pp. 58-69 (Oct. 1972).

Key words: Breakdown starting time; electron avalanche; probabilistic nature of damage; surface damage; wavelength dependence of damage.

Measurements of the laser-induced surface damage process at both ruby and Nd:YAG laser wavelengths are reported in which the laser pulse and beam parameters were carefully held constant for both sources. This resulted in the first directly comparable measurements of laser damage at two different wavelengths. The most striking feature of the data is that all the materials studied are harder to damage at 0.69  $\mu\text{m}$  than at 1.06  $\mu\text{m}$ . In addition, the relationship between the damage probability and the optical electric field strength at 0.69  $\mu\text{m}$ , though similar to that at 1.06  $\mu\text{m}$ , suggests that more than one damage mechanism may be operative.

The probabilistic nature of the laser-induced damage process at 1.06  $\mu\text{m}$  was explored further by measuring the distribution of breakdown starting times with the image-converter streak camera. For a particular laser pulse a threshold-like damage process would result in a very sharp distribution of breakdown starting times. Instead, a large spread is found, with the most likely starting time occurring before the laser intensity reaches its maximum. The observed distribution is described by the compound probability that breakdown occurs at a particular time, given that it has not occurred before that time.

In addition, several possible connections between the probabilistic and threshold-like interpretations of laser-induced damage are discussed. It is shown that these points of view are not totally incompatible.

**Damage to GaAs surfaces from ruby- and Nd-glass laser illumination**, J. L. Smith, *SP372*, pp. 70-74 (Oct. 1972).

Key words: Doping; GaAs; laser induced damage; photoconductivity; surface; surface finish.

Surface damage of GaAs due to 0.694- and 1.06-micron beams from ruby and Nd-glass lasers has been investigated. The wavelengths employed represent photon energies above and below the bandgap of GaAs. For laser operation in the conventional mode, Ga-rich material developed on the surface to a greater extent than for Q-switched operation. Surface damage from Q-switched beams did not appear to depend on the absence, presence, or type of doping, although the nature of the surface preparation was important. The damage threshold for Nd-glass laser illumination was approximately  $10^7 \text{ W/cm}^2$ , only a little higher than that for ruby laser illumination. For Q-switched, Nd-glass laser beam exposure, the damage occurred in highly localized regions and appears to be connected with material flaws near the surface.

**Surface science and surface damage**, J. M. Khan, *SP372*, pp. 75-83 (Oct. 1972).

**Key words:** Laser damage; surface science; thin films.

The relatively new field of Surface Science is concerned with the measurement of physical and chemical properties of well characterized surfaces. The ability to characterize these surfaces has been steadily increasing due to the development of new tools, or the application of older techniques to surface interrogation. The overwhelming result of surface investigation is to draw attention to the difficulty of obtaining such well-characterized surfaces. With this realization in mind, it is highly instructive to review the conventional methods of creating surface conditions. The assumptions involving the conditions at prepared surfaces or interfaces must be reexamined. New procedures may have to be evolved to control conditions to even assure reproducibility. Only when this has been accomplished can measurements of surface damage thresholds be taken as intrinsic characteristics of prepared surfaces.

**Self-focusing with elliptical beams, J. Marburger, *SP372*, pp. 84-91 (Oct. 1972).**

**Key words:** Bulk damage; damage threshold; elliptical beams; enhancement; self-focusing.

The time independent self-focusing of beams whose constant intensity contours are ellipses has been studied in the paraxial ray-constant shape approximation. This approximation leads to equations for the principal  $1/e$  intensity diameters versus axial distance which have been analysed previously by Vorob'yev by a different method. Our method allows the treatment of non-gaussian intensity profiles. The solutions are employed to find expressions for the critical powers and self-focal lengths of nonaxially symmetric beams under a variety of initial conditions. The critical power can be greatly enhanced by astigmatic focusing, even if the beam shape is initially axially symmetric. This theory implies that bulk damage thresholds arising from self-focusing depend strongly on beam shape, in agreement with experimental results of Giuliano.

**Relative contribution of Kerr effect and electrostriction to self-focusing, A. Feldman, D. Horowitz, and R. M. Waxler, *SP372*, pp. 92-99 (Oct. 1972).**

**Key words:** Damage threshold; electrostriction; Kerr-effect; laser damage in glasses; optical glasses; self-focusing.

The ratio of damage thresholds for circularly polarized radiation to linearly polarized radiation was found to be  $> 1$  in borosilicate crown glass, fused silica, and dense flint glass. A Q-switched Nd:glass laser operating in the TEM<sub>00</sub> mode was used. The damage was assumed to result from self-focusing. The fractional contributions of electrostriction and the Kerr effect to the nonlinear index  $n_2$  are estimated from the threshold ratios calculated for each mechanism in the absence of the other and assuming no other self-focusing mechanism. The high damage threshold of fused silica is attributed to its relatively small Kerr effect. Measurements of self-focusing lengths as a function of peak power give qualitatively good agreement with theory.

**Damage measurements with subnanosecond pulses, J. M. McMahon, *SP372*, pp. 100-103 (Oct. 1972).**

**Key words:** Damage mechanisms in laser systems; disc amplifiers; Nd: YAG laser; self-focusing; subnanosecond pulses.

The realization of high energy subnanosecond pulse lasers has been limited by self-focusing damage in laser rods. In this paper measurements on  $n_2$  for laser glasses with subnanosecond pulses are described. The system aspects of

using such glasses are also discussed since in practice this can have a dominant effect on the performance of a high energy short pulse device.

**Time resolved damage studies of thin films and substrate surfaces, J. H. Parks and N. Alyassini, *SP372*, pp. 104-107 (Oct. 1972).**

**Key words:** Damage induced reflectivity change; laser induced damage; laser induced surface acoustic waves; surface; surface breakdown plasma; thin film; time resolved damage.

The time evolution of damage to thin films and substrate surfaces was observed by monitoring the intensity variation of a He-Ne beam reflected from the film or surface during irradiation by a Q-switched ruby laser. Monolayered films including ZnS, CaF<sub>2</sub> and NaCl on fused silica substrates were studied, as well as uncoated fused silica and LiF substrates. When the probe beam is reflected from the exit surface of a substrate sample, the reflected intensity was observed to decrease within the time-scale range of 20-200 nanoseconds to a final value significantly less than that prior to damage. When the probe is spatially offset from the damage region, the reflected intensity decreases and then returns to approximately the predamage value within 0.2-0.3  $\mu$  sec. This reversible effect was observed to be associated with a propagating disturbance on the substrate surface moving with approximately the speed characteristic of a Rayleigh surface wave. The risetime and duration of the plasma which accompanies surface damage was also measured.

The reflected intensity from thin films was observed to increase or decrease depending on the film index of refraction. The monolayer film samples exhibited reflectance changes on the timescale of the ruby pulse, however an offset probe position indicates this change can occur after a time delay of  $\sim 0.1$ - $0.2 \mu$  sec.

**Laser induced damage to mirrors at two pulse durations, E. S. Bliss and D. Milam, *SP372*, pp. 108-122 (Oct. 1972).**

**Key words:** Dielectric mirror; electron avalanche; laser damage mechanisms; laser induced damage; laser monitoring; plasma production; scattering sites.

The damage thresholds of eight, multiple layer dielectric, 95% reflecting mirrors have been measured for single pulses of 20 nanoseconds and 20 picoseconds duration. In both sets of measurements the pulse energy, an oscilloscope trace of the pulse, and the beam's transverse energy density profile at the surface being damaged are recorded for each shot. The variation of the threshold from mirror to mirror and as a function of pulse duration, beam radius, and appearance under microscopic examination is discussed in the context of possible damage mechanisms.

**Study of laser-irradiated thin films, B. E. Newnam and L. G. DeShazer, *SP372*, pp. 123-134 (Oct. 1972).**

**Key words:** Damage morphology; damage thresholds; laser-induced scatter; ruby; spark thresholds; thin films; truncated Gaussian optics.

Laser damage to thin-film coatings was studied using a TEM<sub>00</sub> Q-switched ruby laser. Our study included mono-, bi- and multi-layered coatings of the materials TiO<sub>2</sub>, SiO<sub>2</sub>, ZrO<sub>2</sub>, MgF<sub>2</sub> and ZnS on substrates of glass, rocksalt and spinel. The samples included coatings for antireflection and reflection at the ruby wavelength, and were produced either at USC or by a commercial vendor. Damage threshold energy and power densities were measured with attention paid to dependences on laser beam spot-size, film material and



thickness, substrate condition and incipient scattering of the film. Particular attention was given to the establishment of a threshold criterion for laser damage to thin films. Several effects attendant to damage were investigated, with the conclusion that film scattering induced by the laser was the most sensitive detector of film breakup. The laser induced scatter was observed prior to or at the threshold of spark formation at the film, depending on the film material.

**Influence of structural effects on laser damage thresholds of discrete and inhomogeneous thin films and multilayers,** R. R. Austin, R. C. Michaud, A. H. Guenther, J. M. Putman, and R. Harniman, *SP372*, pp. 135-164 (Oct. 1972).

**Key words:** Laser damage; inhomogeneous films; microscopy; optical coatings; thin film stress.

The dependence of single shot damage threshold on certain film properties is discussed. Variable stress films are produced by mixing components with approximately equal damage thresholds but opposite stress characteristics a definite stress dependence is shown. Films formed from mixtures of high and low threshold components are investigated and found to have damage thresholds between the high and low component values. The damage threshold and damage mode of multilayer and periodic inhomogeneous film systems is compared. The results confirm that the damage threshold is almost entirely material dependent.

**Fundamental absorption mechanisms in high-power laser window materials,** R. Hellwarth, *SP372*, pp. 165-171 (Oct. 1972).

**Key words:** Absorption limit; extrinsic absorption; high-power laser window materials; intrinsic absorption; optical absorption mechanisms; thermal damage.

The thermal deformation and damage to windows and lenses caused by their optical absorption poses serious limitations on the operation of high-power CW and long-pulse lasers. For example, no known materials have both low enough absorption coefficients and good enough mechanical and chemical properties to perform satisfactorily as windows in the large 10.6  $\mu\text{m}$  lasers being developed today. However, very many crystals and glasses would be good candidates for high-power IR windows, if their linear absorption coefficients could be made lower by at least an order of magnitude. Here we review what is known of the physical mechanisms that are responsible for, or may limit, the small residual absorption in the "transparent" wavelength regions of the best candidate window materials. From the primitive state of present knowledge, it seems likely that uncontrolled impurity effects are presently limiting performance in the best window materials, and that therefore their high-power performance can be improved further. We identify theoretical gaps whose filling would greatly improve our understanding of the mechanisms and limits of laser-window absorption.

**Recent developments in high-power infrared-window research,** M. Sparks, *SP372*, pp. 172-175 (Oct. 1972).

**Key words:** Infrared absorption; infrared laser systems; thermal fracture; window materials.

The problem of failure of high-power infrared laser-system windows involves low intensities (a few hundred to a few thousand  $\text{W}/\text{cm}^2$ ). Thermally induced distortion of the optical beam by a heated window and thermal fracture have been considered previously. Pressure-induced optical distortion is discussed. For large-diameter windows of weak materials, the minimum window thickness is determined by

pressure-induced optical distortion, rather than by pressure-induced fracture. Previous figures of merit for rating candidate window materials assumed a constant thickness of 1 cm for all materials. New figures of merit, based on the minimum thickness required to withstand a given pressure, indicate a different preference for materials than that of the previous figures of merit.

It is not known if the measured values of the optical absorption coefficient  $\beta$  for candidate materials are extrinsic or intrinsic. The intrinsic value of  $\beta$  is needed in order to determine if material-improvement programs could produce materials with sufficiently low values of  $\beta$ . Information on extrinsic processes is needed in order to identify the sources of the extrinsic contributions to  $\beta$  so that they may be removed. Measurements of  $\beta$  over ranges of frequency and temperature should be invaluable in obtaining this information. Feasibility studies indicate that emissivity measurements should yield the required values of  $\beta$ , which cannot be obtained by current transmission or calorimetric measurements.

**Low emittance and absorption measurements of windows and mirrors,** G. Wijntjes, N. J. E. Johnson, and J. M. Weinberg, *SP372*, pp. 176-182 (Oct. 1972).

**Key words:** Absorbance measurement; bulk scattering; coating measurement; emittance measurement; infrared absorbance; laser damage.

A cryogenic interferometric spectrometer has been developed which can achieve a noise equivalent spectral radiance (NESR) of  $1.2 \times 10^{-11}$  watts/ $\text{cm}^2\text{-ster-cm}^{-1}$  at 10  $\mu\text{m}$  in 10 seconds of integration, with spectral resolution of 1  $\text{cm}^{-1}$ .

The application of this instrument to the measurement of low level emittance or absorbance in optical elements is described. In such measurements, the specimen is kept at 300 K and its surroundings at 77 K. The measurement is limited by the sensitivity of the instrument, the accuracy of the specimen temperature measurement, and the dynamic range of the measurement. The first limitation is expressed by the noise equivalent spectral emittance.

$$(\text{NE}\Delta\epsilon)_\nu = \frac{\text{NESR}}{R_\nu^0(T)}$$

where  $R_\nu^0(T)$  is the blackbody radiance at temperature  $T$ . With reasonable integration times the determination of emittance is feasible to a precision approaching a part in  $10^7$ , which represents the fundamental limitation to such measurement. The other limitations are proportional to the average emittance over the spectral range considered, and for average emittances below 0.01, permit absolute emittance measurements to a few parts in  $10^6$ . The high spectral resolution of this instrument permits examination of absorption band structure in substrate and coating materials, and the identification of contaminant organic materials. The measurement of bulk scattering in transmissive materials is also possible.

**Investigation of pulsed  $\text{CO}_2$  laser damage of metal and dielectric-coated mirrors,** V. Wang, A. I. Braunstein, M. Braunstein, and J. Y. Wada, *SP372*, pp. 183-193 (Oct. 1972).

**Key words:** Damage mechanisms; inclusions in dielectrics; multilayer dielectric mirrors; pulsed  $\text{CO}_2$  laser damage; thin film coated metal; uncoated metal mirrors.

Recent progress made in pulsed high power  $\text{CO}_2$  lasers has increased the power handling capabilities of mirrors and mirror coatings. Discussed in this paper are surface damage

mechanisms based upon simple physical models (i.e., surface heating, thermally induced stress, absorption centers, etc.) and the experimental results obtained using a pulsed CO<sub>2</sub> laser. Various substrates (Mo, Cu, Ni, quartz, graphite, etc.), metal films (Au, Ag, and Cu), and dielectric coatings (Ge, ThF<sub>4</sub>, CdTe) were exposed to 10.6  $\mu\text{m}$  pulses of 1 to 10  $\mu\text{sec}$  duration with energy fluxes of up to 200 J/cm<sup>2</sup>. The measured threshold values ( $> 140 \text{ J/cm}^2$  for 10  $\mu\text{sec}$  pulses) of polished metal mirrors were generally in agreement with the predicted values based on the simple model. Thin film coated mirrors exhibited slightly lower threshold values ( $\approx 75$  to  $140 \text{ J/cm}^2$  for 10  $\mu\text{sec}$  pulses) than that of simple metal metals. The thresholds for those limited numbers of dielectric mirrors tested were even lower ( $\approx 10 \text{ J/cm}^2$  for pulses of 1 to 10  $\mu\text{sec}$  lengths); this low performance is attributed to inclusions which act as local absorption centers within the dielectric.

**SP373. Bibliography of temperature measurement, January 1953 to December 1969, P. D. Freeze and L. P. Parker, Nat. Bur. Stand. (U.S.), Spec. Publ. 373, 140 pages (Nov. 1972).**

Key words: Fluidic thermometers; pyrometry; radiation pyrometry; temperature measurement; thermistors; thermocouple; thermometry.

This bibliography consolidates into a single publication National Bureau of Standards Monograph 27 (January 1953 to June

1960) and its two supplements (September 13, 1963 and April 28, 1967, respectively) together with 1800 new references covering essentially the period from January 1966 to December 1969, but including some earlier citations previously omitted. The consolidated publication, which supersedes the earlier bibliographies, thus covers literature of temperature measurement published between January 1953 and December 1969.

In general, the arrangement of material in this new edition is the same as in Monograph 27, and the journal abbreviations are those employed in Chemical Abstracts. However, starting with 1963, and in the new material, scope of coverage in Part 1 was broadened to include theory, calibration, and temperature scales in addition to the previous categories of thermoelectric theory and calibration.

**SP376. Ruler: 15 cm/6 in, with metric-customary units and equivalents, Nat. Bur. Stand. (U.S.), SP367, Both Sides (Dec. 1972).**

Key words: Centimeter; conversion; customary units; inch; metric units.

This ruler provides metric linear measure (15 cm) and customary-unit linear equivalents (approximately 6 inches) plus conversion formula for effecting changes from customary to metric units.



### 3.7. APPLIED MATHEMATICS SERIES

Mathematical tables, manuals, and studies of special interest to physicists, engineers, chemists, biologists, mathematicians, computer programmers and others engaged in scientific and technical work. Some of the volumes are reissues of the Mathematical Tables prepared by the Project for the Computation of Mathematical Tables conducted by the Works Projects Administration for the city of New York under the scientific sponsorship of NBS.

AMS62. *Cyclic designs*, J. A. John, F. W. Wolock, H. A. David, J. M. Cameron, and J. A. Speckman, Nat. Bur. Stand. (U.S.), Appl. Math. Ser. 62, 79 pages (Apr. 1972).

Key words: Analysis of variance; cyclic designs; design of

experiments; designs for calibration; incomplete block designs.

Cyclic designs are incomplete block designs based on cyclic development of an initial block or blocks. Their flexibility, ease in conduct of the experiment and natural grouping for elimination of heterogeneity make them worthy of attention in their own right even though their analysis does not possess the ease of computation of the more common completely balanced or partially balanced incomplete block designs with two associate classes. Methods for construction and analysis of the designs are given along with a numerical example. Applications of the designs are discussed and an appendix on their use in calibration is given.

### 3.8. NATIONAL STANDARD REFERENCE DATA SERIES

Includes the evaluated reference data and critical reviews of long-term interest that are produced by data centers within the NSRDS network. The National Standard Reference Data System is a Government-wide effort to provide the U.S. technical community with effective access to the quantitative data of physical science, critically evaluated and compiled for convenience.

NSRDS-NBS3. Section 5. In Press.

NSRDS-NBS3. Section 6. Selected tables of atomic spectra: A. Atomic energy levels—second edition; B. Multiplet tables, H<sub>1</sub>, D, T (Data derived from the analyses of optical spectra), C. E. Moore and E. O. Hulburt, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 3, Sec. 6, 36 pages (Sept. 1972).

Key words: Atomic energy levels, H<sub>1</sub>, D, T; hydrogen spectra, H<sub>1</sub>, D, T; multiplet tables, H<sub>1</sub>, D, T; spectra H<sub>1</sub>, D, T; wavelengths, hydrogen spectra H<sub>1</sub>, D, T.

The present publication is the sixth Section of a series being prepared in response to the persistent need for a current revision of two sets of tables containing data on atomic spectra as derived from analyses of optical spectra. As in the previous sections, Part A contains the atomic energy levels and Part B the multiplet tables. The spectra of hydrogen and of the isotopes deuterium and tritium are included. The form of presentation is described in detail in the text to Section 1.

NSRDS-NBS35. Volume I. Atomic energy levels as derived from the analyses of optical spectra, <sup>1</sup>H to <sup>23</sup>V, C. E. Moore, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 35/V.I, 359 pages (Dec. 1971).

Key words: Energy levels; H-V.

This series of three volumes is a critical compilation of atomic energy levels prepared at the National Bureau of Standards from the analyses of optical spectra. Volume I contains data on the spectra of hydrogen, deuterium, tritium, helium, lithium, beryllium, boron, carbon, nitrogen, oxygen, fluorine, neon, sodium, magnesium, aluminum, silicon, phosphorus, sulfur, chlorine, argon, potassium, calcium, scandium, titanium, and vanadium (<sup>1</sup>H to <sup>23</sup>V). Volume II covers the spectra of chromium, manganese, iron, cobalt, nickel, copper, zinc, gallium, germanium, arsenic, selenium, bromine, krypton, rubidium, strontium, yttrium, zirconium, and niobium (<sup>24</sup>Cr to <sup>41</sup>Nb). Volume III includes the spectra of molybdenum, technetium, ruthenium, rhodium, palladium, silver, cadmium, indium, tin, antimony, tellurium, iodine, xenon, cesium, barium, lanthanum; hafnium, tantalum, tungsten, rhenium, osmium, iridium, platinum, gold, mercury, thallium, lead, bismuth, polonium, radon, radium, and actinium (<sup>42</sup>Mo to <sup>57</sup>La; <sup>72</sup>Hf to <sup>89</sup>Ac). This is a reprint of NBS Circular 467, Volume I.

NSRDS-NBS35. Volume II. Atomic energy levels as derived from the analyses of optical spectra, <sup>24</sup>Cr to <sup>41</sup>Nb, C. E. Moore, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 35/V.II, 259 pages (Dec. 1971).

Key words: Cr-Nb; energy levels.

This series of three volumes is a critical compilation of atomic energy levels prepared at the National Bureau of Standards from the analyses of optical spectra. Volume I contains data on the spectra of hydrogen, deuterium, tritium, helium, lithium, beryllium, boron, carbon, nitrogen, oxygen, fluorine, neon, sodium,

magnesium, aluminum, silicon, phosphorus, sulfur, chlorine, argon, potassium, calcium, scandium, titanium, and vanadium (<sup>1</sup>H to <sup>23</sup>V). Volume II covers the spectra of chromium, manganese, iron, cobalt, nickel, copper, zinc, gallium, germanium, arsenic, selenium, bromine, krypton, rubidium, strontium, yttrium, zirconium, and niobium (<sup>24</sup>Cr to <sup>41</sup>Nb). Volume III includes the spectra of molybdenum, technetium, ruthenium, rhodium, palladium, silver, cadmium, indium, tin, antimony, tellurium, iodine, xenon, cesium, barium, lanthanum; hafnium, tantalum, tungsten, rhenium, osmium, iridium, platinum, gold, mercury, thallium, lead, bismuth, polonium, radon, radium, and actinium (<sup>42</sup>Mo to <sup>57</sup>La; <sup>72</sup>Hf to <sup>89</sup>Ac). This is a reprint of NBS Circular 467, Volume II.

NSRDS-NBS35. Volume III. Atomic energy levels as derived from the analyses of optical spectra, <sup>42</sup>Mo to <sup>57</sup>La, <sup>72</sup>Hf to <sup>89</sup>Ac, C. E. Moore, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 35/V.III, 282 pages (Dec. 1971).

Key words: Energy levels; Hf-Ac; Mo-La.

This series of three volumes is a critical compilation of atomic energy levels prepared at the National Bureau of Standards from the analyses of optical spectra. Volume I contains data on the spectra of hydrogen, deuterium, tritium, helium, lithium, beryllium, boron, carbon, nitrogen, oxygen, fluorine, neon, sodium, magnesium, aluminum, silicon, phosphorus, sulfur, chlorine, argon, potassium, calcium, scandium, titanium, and vanadium (<sup>1</sup>H to <sup>23</sup>V). Volume II covers the spectra of chromium, manganese, iron, cobalt, nickel, copper, zinc, gallium, germanium, arsenic, selenium, bromine, krypton, rubidium, strontium, yttrium, zirconium, and niobium (<sup>24</sup>Cr to <sup>41</sup>Nb). Volume III includes the spectra of molybdenum, technetium, ruthenium, rhodium, palladium, silver, cadmium, indium, tin, antimony, tellurium, iodine, xenon, cesium, barium, lanthanum; hafnium, tantalum, tungsten, rhenium, osmium, iridium, platinum, gold, mercury, thallium, lead, bismuth, polonium, radon, radium, and actinium (<sup>42</sup>Mo to <sup>57</sup>La, <sup>72</sup>Hf to <sup>89</sup>Ac). This is a reprint of NBS Circular 467, Volume III.

NSRDS-NBS39. Tables of molecular vibrational frequencies, consolidated Volume I, T. Shimanouchi, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 39, 164 pages (June 1972).

Key words: Fundamental frequencies; infrared spectra; polyatomic molecules; Raman spectra; vibrational frequencies.

The compilations of fundamental vibrational frequencies of molecules previously published as NSRDS-NBS6, NSRDS-NBS11, and NSRDS-NBS17 have been revised and extended to 52 additional molecules. This consolidated volume includes data on a total of 223 molecules. Selected values of the fundamental vibrational frequencies are given for each molecule, together with observed infrared and Raman spectral data and citations to the original literature. The selection of vibrational fundamentals has been based on careful studies of the spectral data and comprehensive normal-coordinate analyses. An estimate of the accuracy of the selected values is included. The tables provide a convenient source of information for those who require vibrational energy levels and related properties in molecular spectroscopy, thermodynamics, analytical chemistry, and other fields of physics and chemistry.

NSRDS-NBS40. A multiplet table of astrophysical interest, (Revised Edition), Part I—Table of multiplets and Part II—



**Finding list of all lines in the table of multiplets**, C. E. Moore, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 40, 253 pages (Feb. 1972).

Key words: Atomic spectra, multiplet table; finding list, atomic spectra; multiplet table; spectra, atomic.

Pending the completion of a current edition, the 1945 Multiplet Table is being reprinted here to meet continuing demands. The leading lines in 196 atomic spectra of 85 chemical elements are listed in related groups called multiplets. Estimated intensities, excitation potentials and multiplet designations are given for the individual lines, and each multiplet is assigned a number. An extensive bibliography covers the source material used for the compilation.

The Table is presented in two parts: Part I includes the multiplets, with the spectra of each element being given in order of increasing ionization, and the elements in order of increasing atomic number. Part II is a Finding List in which all the lines in Part I are entered in order of increasing wavelength, with their multiplet numbers.

The range of the Table is from 2951 Å to 13164 Å. A supplementary table of "Forbidden Lines" extends from 2972 Å to 12645 Å. Reprint of NBS Technical Note 36 (PB151395).

**NSRDS-NBS41. Crystal structure transformations in binary halides**, C. N. R. Rao and M. Natarajan, Nat. Stand Ref. Data Ser., Nat. Bur. Stand. (U.S.), 41, 53 pages (July 1972).

Key words: Binary halides; crystal structure transformation; electronic data; phase transformation; spectroscopic data; thermodynamic data; x-ray diffraction data.

A critical survey of the data describing crystal structure transformations in binary halides is compiled. Data on thermodynamic, crystallographic, spectroscopic and electronic properties are given for each transformation. Experimental techniques used to obtain the data are named and comments on the data are included in the tables. The literature is surveyed up to 1970. References have been selected on the basis of their pertinence to the data which are cited and do not represent all the available literature.

**NSRDS-NBS42. Selected specific rates of reactions of the solvated electron in alcohols**, E. Watson, Jr., and S. Roy, Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 42, 22 pages (Aug. 1972).

Key words: Alcohols; chemical kinetics; data compilation; radiation chemistry; rates; solvated electron.

Solvated electrons are generated in alcohols by radiolysis, photolysis, reaction with sodium, etc. Rates of reactions of  $e_s^-$  with solvent and solute molecules, ions, and transients, in alcohol solutions, have been compiled. Arrhenius parameters are tabulated for some reactions.

### 3.9. BUILDING SCIENCE SERIES

Disseminates technical information developed at the Bureau on building materials, components, systems, and whole structures. The series presents research results, test methods, and performance criteria related to the structural and environmental functions and the durability and safety characteristics of building elements and systems.

These publications, similar in style and content to the NBS Building Materials and Structure Reports (1938-59), are directed toward the manufacturing, design, and construction segments of the building industry, standards organizations, officials responsible for building codes, and scientists and engineers concerned with the properties of building materials.

**BSS39. Use of computers for environmental engineering related to buildings.** Proceedings of a Symposium sponsored by the National Bureau of Standards, the American Society of Heating, Refrigerating and Air-Conditioning Engineers, Inc., and the Automated Procedures for Engineering Consultants, Inc., held at the National Bureau of Standards, Gaithersburg, Md., Nov. 30-Dec. 2, 1970, T. Kusuda, Editor, Nat. Bur. Stand. (U.S.), Bldg. Sci. Ser. 39, 826 pages (Sept. 1971).

Key words: Building heat transfer analysis; energy usage; environmental engineering; heating and air conditioning; use of computers.

This proceedings of the First Symposium on the Use of Computers for Environmental Engineering Related to Buildings contains all of the technical papers and invited addresses presented at the symposium, which was held November 30-December 2, 1970, at the National Bureau of Standards.

The fifty-nine papers deal with the application of the computer to such environmental engineering problems as building heat transfer calculations, heating and cooling load calculations, system simulations, energy usage analyses, computer graphics, air and smoke movement inside buildings, and weather data analyses for load and energy usage calculations.

**BSS41. Performance of a single-stack DWV system utilizing low-angle stack-branch confluence and bottom shunt venting,** R. S. Wyly and G. C. Sherlin, Nat. Bur. Stand. (U.S.), Bldg. Sci. Ser. 41, 24 pages (Apr. 1972).

Key words: Criteria for plumbing; hydraulic test loads; performance of plumbing; single stack plumbing.

Among the more important criteria for hydraulic and pneumatic performance of sanitary drain-waste-vent systems are (1) maintenance of water seals in fixture traps, (2) limitation of pneumatic pressures, (3) limitation of hydrostatic and hydrodynamic

pressures, and (4) limitation of cross-flow between horizontal branches or trap arms.

Recent tests of a single-stack drainage system proposed for a high-rise apartment project in Fairfax County, Virginia have produced the following findings with respect to these performance criteria: (1) test loads (total discharge rates) ranging up to magnitudes greater than predicted loads yielded reasonable average trap-seal retention; (2) the use of trap-seal retention as a measure of performance appears to be more meaningful than the traditional pneumatic-pressure measure; (3) fitting geometry and branch arrangement can be more critical in single-stack systems than in conventional vented systems, and (4) present procedures for selecting test loads, for making tests, and for reporting and interpreting measured values need improvement and standardization.

**BSS42. Design loads for inserts embedded in concrete,** T. W. Reichard, E. F. Carpenter, and E. V. Leyendecker, Nat. Bur. Stand. (U.S.), Bldg. Sci. Ser. 42, 28 pages (May 1972).

Key words: Anchors; concrete slabs; design loads; fatigue; inserts; pull-out loads; sustained load.

Detailed test procedures are presented for a research program on cast-in-place inserts embedded in reinforced concrete. Three types of inserts, two of malleable iron and one of ductile steel, capable of receiving a 3/4 inch threaded rod were tested. Other variables included concrete aggregate type, concrete strength, reinforcement cover and spacing, angular loading, flexural cracking, sustained load and fatigue loading.

It was found that the pull-out load for an insert could be approximated by a linear function of the concrete unit weight and square root of the compressive strength in a statically loaded reinforced concrete slab. The effect of other variables is related to the insert pull-out loads in these slabs. Design recommendations are presented.

**BSS43. Paper honeycomb sandwich panels as lightweight structural components,** T. W. Reichard, Nat. Bur. Stand. (U.S.), Bldg. Sci. Ser. 43, 7 pages (Apr. 1972).

Key words: Adhesives; paper honeycomb; sandwich facings; sandwich panels.

This paper presents a resume of current practice in the U.S. with regard to the use of sandwich panels in single-story buildings. A description and the properties of typical paper honeycomb cores are given. Some of the factors which are considered in choosing sandwich facings and adhesives are given.



### 3.10. FEDERAL INFORMATION PROCESSING STANDARDS PUBLICATIONS

The publications in this series collectively constitute the Federal Information Processing Standards Register. The purpose of the Register is to serve as the official source of information in the Federal Government regarding (1) uniform Federal information processing standards resulting from provisions of Public Law 89-306 (the Brooks Bill), and (2) data elements and codes standards in data systems developed under the provisions of Bureau of the Budget Circular No. A-86. FIPS PUBS will include approved Federal Information Processing Standards information of general interest, and a complete index of relevant standards publications.

**FIPS PUB 8-2. Standard metropolitan statistical areas**, H. E. McEwen, Standards Coordinator, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS Pub.) 8-2, 17 pages (1972).

**Key words:** Computers; data processing; Federal Information Processing Standards Publication; representations and codes; Standard Metropolitan Statistical Areas.

This publication provides standard identifications and codes for representing Standard Metropolitan Statistical Areas for the interchange of machine sensible data among agencies. It supersedes FIPS PUB 8-1, Metropolitan Statistical Areas, dated July 1, 1971. The general concept of a Standard Metropolitan Statistical Area, commonly referred to as "SMSA," is one of an integrated economic and social unit with a recognized large population nucleus.

**FIPS PUB 12-1. Federal information processing standards index**, H. E. McEwen, Standards Coordinator, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS Pub.) 12-1, 140 pages (1972).

**Key words:** American National Standards; computers, data elements and codes; data processing systems; Federal Information Processing Standards; International Organization for Standardization; management information systems; U.S. Government.

This publication provides material concerning standardization activities in the area of information processing at the Federal, National and International levels. Also included are related policy and procedural guideline documents. A list of Federal Government participants involved in the development of Federal Information Processing Standards is provided. This FIPS PUB is revised and updated annually. Supersedes NBS FIPS PUB 12.

**FIPS PUB 20. Guidelines for describing information interchange formats**, H. S. White, Jr., Standards Coordinator, Nat. Bur.

Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS Pub.) 20, 11 pages (1972).

**Key words:** Data processing systems standards; Federal Information Processing Standards; formatted records; information interchange; United States Government.

This publication provides guidelines which identify and describe the various characteristics of formatted information that should be considered whenever formatted information is interchanged. The objective is to clarify and improve the documentation necessary to effectively provide, process, or use the information involved. The guidelines provided are to be used throughout the Federal Government as a checklist for preparing effective documentation of formatted information interchange.

**FIPS PUB 21. Common business oriented language COBOL**, R. R. Roundtree, Standards Coordinator, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS Pub.) 21, 4 pages (1972).

**Key words:** COBOL; data processing; Federal Information Processing Standard; information interchange; information processing; programming language; software.

This FIPS PUB announces the adoption of the American National Standard COBOL (X3.23-1968) as the Federal Standard COBOL. The American National Standard defines the elements of the COBOL Programming Language and the rules for their use. The standard is used by implementors as the reference authority in developing compilers and by users for writing programs in COBOL. A primary purpose of the standard is to promote a high degree of interchangeability of programs for use on a variety of automatic data processing systems.

The COBOL language is intended for use with business-oriented applications.

**FIPS PUB 22. Synchronous signaling rates between data terminal and data communication equipment**, G. E. Clark, Jr., Standards Coordinator, Nat. Bur. Stand. (U.S.), Fed. Info. Process. Stand. Publ. (FIPS Pub.) 22, 4 pages (1972).

**Key words:** Data communication equipment; data processing terminal equipment; data transmission (voice band); Federal Information Processing Standards; synchronous signaling rates; teleprocessing.

This publication prescribes speeds for transferring binary encoded information in synchronous serial or parallel forms between data terminal and data communication equipment employing voice band communication facilities. Speeds ranging from 75 to 9600 bits-per-second are specified.

### 3.11. PRODUCT STANDARDS

This series comprises voluntary standards that establish (1) dimensional requirements for standard size and types of various products, (2) technical requirements for the product, and (3) methods of testing, grading, and marking these products. The objective is to define requirements for products in accordance with the principal demands of the trade.

**PS45-71. Body measurements for the sizing of apparel for young men (students),** C. W. Devereux, Technical Standards Coordinator, Nat. Bur. Stand. (U.S.), Prod. Stand. 45-71, 16 pages (Jan. 1972).

Key words: Apparel, young men's (students'); body measurements, young men's (students'); classification, young men's (students') size; grading charts, young men's (students') size; size designations, young men's (students').

This Voluntary Product Standard covers size categories, size designations, and body measurements for the sizing of apparel for boys designated young men or students. The young men (students) category is intended to include those boys and young men who have achieved most of their adult height, but not adult girth. The Standard includes the following: applications of the body sizing system, methods of measuring the body, an explanation of the development of the Standard (appendix A) and sizing grades (appendix B). Also included is a method of identifying products that are sized using the measurements and designations in the Standard.

**PS51-71. Hardwood and decorative plywood,** P. R. Sutula, Technical Standards Coordinator, Nat. Bur. Stand. (U.S.), Prod. Stand. 51-71, 18 pages (Jan. 1972).

Key words: Decorative plywood; hardwood plywood; plywood, hardwood and decorative; softwood plywood, decorative; veneer grades, decorative softwood and hardwood.

This Voluntary Product Standard for hardwood and decorative plywood establishes the nationally recognized marketing classifications, quality criteria, test methods, definitions, and grade-marking and certification practices for plywood produced primarily from hardwoods. It is intended for voluntary use by reference in trade literature, catalogs, sales contracts, building codes, and procurement specifications to describe the quality aspects of the product and the means to determine conformance.

Requirements are given for wood species, veneer grading, lumber-core, particleboard-core, hardboard-core, glue bond, panel constructions, dimensions, moisture content, sanding, and finishing. Sampling and testing provisions cover dry shear, cyclic-boil, three cycle wet and dry, and cold soak test methods for plywood delamination determinations, and field and laboratory

moisture content measuring methods. A glossary of trade terms is provided for better communication and understanding, and provisions are made for panel grade-marking and certification to indicate compliance. Supersedes NBS CS 35-61.

**PS52-71. Polytetrafluoroethylene (PTFE) plastic tubing,** L. H. Breden, Technical Standards Coordinator, Nat. Bur. Stand. (U.S.), Prod. Stand. 52-71, 12 pages (Apr. 1972).

Key words: Chemical, mechanical, and electrical tubing; fluorocarbon plastic tubing; plastic tubing, polytetrafluoroethylene; PTFE tubing; tubing, PTFE-fluorocarbon.

This Voluntary Product Standard covers commercially available PTFE tubing intended for chemical, mechanical, and electrical applications. Included are requirements and methods of test for materials, dimensions, and physical and chemical properties. A method for identifying products which comply with this Standard is provided.

**PS53-72. Glass-fiber reinforced polyester structural plastic panels,** L. H. Breden, Technical Standards Coordinator, Nat. Bur. Stand. (U.S.), Prod. Stand. 53-72, 13 pages (Apr. 1972).

Key words: Glass-fiber reinforced polyester panels; panels, glass-fiber reinforced polyester; plastic panels, structural; structural panels.

This Voluntary Product Standard covers two types of plastic panels furnished in three weights and seven geometrical configurations, including flat panels, intended for use in structural applications. The Standard covers requirements for the sizes, configurations, weights, and squareness of the panels. Included are requirements for materials, appearance, color uniformity, light transmission, transverse load, bearing load, flammability, packing, and marking. Methods for identifying products that conform to this Standard are also included. Information on chemical resistance and available panels is provided in an appendix.

**PS55-72. Rigid poly (vinyl chloride) (PVC) plastic siding,** L. H. Breden, Technical Standards Coordinator, Nat. Bur. Stand. (U.S.), Prod. Stand. 55-72, 11 pages (Nov. 1972).

Key words: Building materials; flammability of outdoor siding; plastic material; poly (vinyl chloride) siding; siding, poly (vinyl chloride); weathering of plastic siding.

This Voluntary Product Standard establishes requirements and methods of test for the materials, dimensions, weight, warp, shrinkage, flammability, impact strength, weatherability, expansion, and appearance of extruded single wall siding, manufactured from rigid PVC compound. Methods of indicating compliance with this Standard are also provided.



### 3.12. TECHNICAL NOTES

Designed to supplement the Bureau's regular publications program, Technical Notes provide a publication medium for communications and reports on data of limited or transitory interest. They often serve as final reports on work sponsored at NBS by other Government agencies.

**TN379-1. Standard time and frequency: its generation, control, and dissemination from the National Bureau of Standards Time and Frequency Division,** J. B. Milton, Nat. Bur. Stand. (U.S.), Tech. Note 379-1, 26 pages (June 1972).

**Key words:** Clock synchronization; frequency and time dissemination; primary frequency standard; standard frequency broadcasts; time interval; time scales.

The Time and Frequency Division of the National Bureau of Standards produces the NBS time scales, AT(NBS) and UTC(NBS). These time scales are developed by utilizing the properties of the NBS frequency standard, NBSFS. The main byproduct of these time scales is the operational clock systems. These operational clock systems are used, among other things, to calibrate the clocks and secondary standards necessary for the operation of the NBS radio stations, WWV, WWVB, WWVL, and WWVH. These stations transmit UTC(NBS), and various tones, alerts, and corrections for time-of-day information.

**TN467. Activation analysis: a bibliography through 1971,** G. J. Lutz, R. J. Boreni, R. S. Maddock, and J. Wing, Editors, Nat. Bur. Stand. (U.S.), Tech. Note 467, 892 pages (Aug. 1972).

**Key words:** Activation analysis; bibliography; element determined; literature file; matrix analyzed; technique used.

References to papers published in the open literature which describe work using activation analysis are printed from a computer based storage and retrieval system. Published as a two-part volume, part 1 is a listing of references according to accession numbers (approximately 6200) while part 2 is composed of four appendices. Appendix I is an index for the element determined, Appendix II is an index of the matrix analyzed, Appendix III is an index of the technique used, Appendix IV is an author index. The two parts when used together, permit a literature search defined by the several indices. Supersedes NBS TN467, Parts 1 and 2 issued May 1971.

**TN582. Activities of the NBS Spectrochemical Analysis Section, July 1970 to June 1971,** K. F. J. Heinrich and S. D. Rasberry, Nat. Bur. Stand. (U.S.), Tech. Note 582, 126 pages (Jan. 1972).

**Key words:** Analysis; computer program; electron probe; microanalysis; optical spectrometry; pre-concentration techniques; spectrochemical analysis; standard reference materials; x-ray fluorescence analysis.

Spectrochemical research activities, improvements in equipment and applications, especially to the certification of NBS Standard Reference Materials, are summarized. In optical emission spectroscopy, studies have been carried out on a modified gas-sheath arc excitation source. Application has been made of this source and several other conventional excitation sources to analytical problems related to both standard reference materials and other materials being investigated at NBS. Newly derived computation procedures for quantitative x-ray fluorescence analysis are described as well as new instrumentation added for x-ray spectrochemical studies. In electron probe microanalysis, research and new instrumentation has been directed to improved

detection limits and quantitation; special emphasis has been given to methods for small particles and biological thin cuts. Methods of pre-concentration of impurities have been advanced and applied, in some cases at parts per billion ( $10^{-9}$ ) limits, to water pollution, river sediment specimens. Mercury, cadmium, and lead were among the elements determined. Work on Standard Reference Materials resulted in certification of several special steels, several high temperature alloys, a high-silicon steel and a titanium alloy, among others. Listings are given of 8 publications and 25 talks by members of the Section during the year.

**TN585. Microchemical Analysis Section: Summary of activities, July 1970 to June 1971,** J. K. Taylor, Editor, Nat. Bur. Stand. (U.S.), Tech. Note 585, 77 pages (Jan. 1972).

**Key words:** Air pollution analysis; carbon monoxide; fire research; microchemical analysis; nitrogen dioxide; ozone; particulate analysis; sulfur dioxide.

This report describes the scientific program of the Microchemical Analysis Section of the Analytical Chemistry Division of the National Bureau of Standards, Institute for Materials Research during July 1970 to June 1971. General activities are reported in the areas of air pollution measurement standards including both gases and particulates, in the field of microchemical analysis, in fire research and in electrochemical analysis performed under an international research grant program. A sulfur dioxide standard reference material for use in monitoring ambient atmosphere, and the initial work on a similar standard for stationery sources are described. Research activities on potential standard reference materials for ozone, nitrogen dioxide, and carbon monoxide are also described.

**TN587. Organic Chemistry Section: Summary of activities, July 1970 to June 1971,** R. Schaffer, Editor, Nat. Bur. Stand. (U.S.), Tech. Note 587, 131 pages (Aug. 1972).

**Key words:** Bilirubin; cholesterol; cortisol; e.s.r.; D-mannitol; NADH; n.m.r.; purity; SRM; Standard Reference Materials; VMA.

This report of the Organic Chemistry Section of the National Bureau of Standard's Institute for Materials Research provides a summary of a year's scientific activity; as such, it covers both work that was completed and some that is still in progress. The development of Standard Reference Materials (SRM's) and their certification, and journal publications describing aspects of that work, as well as other research activities, are the output of the Section.

In the SRM category, the major subjects of this report are bilirubin, cholesterol, cortisol, D-glucose, 4-hydroxy-3-methoxy-DL-mandelic acid (VMA), D-mannitol, and the reduced form of nicotinamide adenine dinucleotide (NADH).

Studies concerning carbohydrates include synthetic work with D-psicose, n.m.r. employing internuclear double-resonance, and mass spectroscopy of 6-deoxy-1,2:3,5-di-O-isopropylidene- $\alpha$ -D-glucose, spectroscopic studies of derivatives of 6-amino-6-deoxy-D-glucose-6- $^{15}\text{N}$  (employing mass spectrometry, Fourier-transform,  $^{13}\text{C}$ -n.m.r. and heteronuclear,  $^{15}\text{N}$  indor techniques), and *p*-bromophenylosotriazoles of inositols.

Other research utilized e.s.r. and involved periodic acid oxidation of azines, solid-state oxidation of benzenehexol on active manganese dioxide, and the formation of stable radical-anions from glyoxal bis(phenylhydrazone).

TN593. Wire-bond electrical connections: testing, fabrication and degradation-A bibliography 1957-1971, H. A. Schafft, Nat. Bur. Stand. (U.S.), Tech. Note 593, 58 pages (Jan. 1972).

Key words: Bibliography; degradation (wire-bond); discrete devices; electrical interconnection; fabrication (wire-bond); failure (wire-bond); hybrid circuits; integrated circuits; microelectronics; reliability; testing (wire-bond); wire-bond.

More than 245 papers relevant to wire-bond type electrical interconnections used in microelectronic and low-power discrete and hybrid devices are listed together with key words. The bibliographic search concentrated on compiling papers which appeared in the period from 1965 to 1970, inclusive. The selection of papers was generally limited to those that were pertinent to wire-bonds where the wire diameter is less than about 50  $\mu\text{m}$  (2 mils) and where the wire is bonded by either thermocompressive or ultrasonic means. Two indexes are provided: (1) an Author Index and (2) a Key Word Index. The latter includes a tabulation of the literature citations.

TN594-1. Optical radiation measurements: Fundamental principles of absolute radiometry and the philosophy of this NBS program (1968 to 1971), J. Geist, Nat. Bur. Stand. (U.S.), Tech. Note 594-1, 59 pages (June 1972).

Key words: Absolute detector radiometry; electrically calibrated detectors; International Pyrheliometric Scale; irradiance; radiometry.

The philosophy of the present NBS program in realizing a scale of total irradiance with electrically calibrated (absolute) detectors, a theoretical analysis of the sources of error in such a scale realization, a description of the electrically calibrated detector developed from 1968 to 1971, and participation in the Third International Pyrheliometer Comparison are presented.

TN594-2. Optical radiation measurements: Photometric instrumentation and research (1970 to 1971), E. F. Zalewski, A. R. Schaefer, K. Mohan, and D. A. McSparron, Nat. Bur. Stand. (U.S.), Tech. Note 594-2, 44 pages (Sept. 1972).

Key words: Instrumentation; lamp orientation; lamp power circuitry; lamp stability; photodetector amplifier; photometry.

This document was written primarily to serve two purposes. First, some of the basic instrumentation which has recently been developed for use in photometry at NBS is described. The design and application of photodetector amplifiers, lamp power circuitry, and mechanical instrumentation are discussed. Second, three photometric experiments are described: the stability testing of some flux lamps and intensity lamps and the determination of the dependence of relative intensity on orientation. These experiments and their conclusions have proven useful in pointing out areas which need further investigation and in planning the directions of future work.

TN594-3. Optical radiation measurements: Photometric calibration procedures, V. I. Burns and D. A. McSparron, Nat. Bur. Stand. (U.S.), Tech. Note 594-3, 35 pages (Nov. 1972).

Key words: Calibration procedures; color temperatures; luminous flux; luminous intensity; photometry; uncertainty.

The National Bureau of Standards supplies calibrations of luminous intensity, luminous flux and color temperature on a routine basis. The procedures, equipment, and techniques used to perform these calibrations as of October 1972 are described. Details of the uncertainty information currently available, including estimates and procedures for determining uncertainties of the reported values, are also presented.

TN610. Application of VLF theory to time dissemination, W. F.

Hamilton and J. L. Jespersen, Nat. Bur. Stand. (U.S.), Tech. Note 610, 170 pages (Nov. 1971).

Key words: Diurnal phase; Omega; time; time dissemination; VLF propagation; zonal harmonics.

The characteristics of time dissemination systems are discussed. Particular emphasis is placed on the advantages and problems of very low frequency (VLF) timing systems. The parameters affecting VLF propagation along with causes of variations in these parameters, are discussed. Three methods of computing VLF propagation delays—mode theory, geometric-optics, and zonal harmonics—are compared. The method of zonal harmonics, used for the calculations in this paper, is discussed in more detail. A method of calculating reflection coefficients for a continuously varying ionosphere is described. The theoretical values are compared with experimental measurements. Graphical results of the calculations are included.

TN611. NBS frequency-time broadcast station WWV, Fort Collins, Colo., P. P. Viezbicke, Nat. Bur. Stand. (U.S.), Tech. Note 611, 29 pages (Oct. 1971).

Key words: High frequency; standard radio frequencies; time-frequency broadcasts; time signals; WWV.

This report describes the design and construction of the National Bureau of Standards frequency-time broadcast station located at Fort Collins, Colo. The principal function of the station is to broadcast basic standards of frequency and time signals on frequencies of 2.5, 5, 10, 15, 20, and 25 MHz. These high frequency transmissions, which can be received on the simplest of equipment, provide the necessary accuracy required to fulfill some of the needs of industry, Government, and the public. The technical and administrative supervision of the station is under the Time and Frequency-Time Broadcast Services Section, National Bureau of Standards, Boulder, Colo.

TN612. Frequency shifts due to Ramsey type interrogation in atomic beam tubes, H. Hellwig, J. A. Barnes, D. J. Glaze, and P. Kartaschoff, Nat. Bur. Stand. (U.S.), Tech. Note 612, 25 pages (Feb. 1972).

Key words: Cavity phase shift; cesium beam tube; frequency accuracy; frequency standard; power shift; resonance line shape.

*Part I:* A phase difference between the two interaction regions of a Ramsey excitation resonance structure results in a frequency bias in the measured beam resonance. A simple mathematical model is discussed which describes the dependence of this bias on the phase difference, the microwave power level, the modulation amplitude, and the resonance linewidth. This dependence results from the interaction of the modulated microwave excitation frequency with the asymmetric shape of the slightly shifted resonance line. In a first order approximation, no dependency on the frequency modulation amplitude is expected. Near-linear dependencies on the linewidth and microwave power level which are quite pronounced even at relatively small cavity phase differences are predicted. The theoretical results are compared with one set of experimental data on the microwave power dependence as measured in 1969 with the primary cesium beam standard NBS-III. After a correction is applied to remove the power dependence due to spectral impurity of the microwave excitation, the remaining measured power dependence agrees quantitatively with that calculated using a cavity phase difference of about 3 milliradians.

*Part II:* One of the most serious effects limiting the accuracy of atomic beam resonators is the uncertainty of phase shifts between the oscillating fields in a Ramsey excitation cavity. A technique using the linewidth dependence on the excitation



power to measure the phase-shift induced bias has recently been proposed. The conditions under which this method is valid and their implications on the design of beam optics will be discussed with consideration of available experimental results.

**TN614. Longitudinal magnetoresistance in polar semiconductors,** R. L. Peterson, Nat. Bur. Stand. (U.S.), Tech. Note 614, 47 pages (Apr. 1972).

Key words: Magnetophonon effect; magnetoresistance; semiconductors; transport theory.

The magnetophonon effect due to resonant interactions of charge carriers with optical phonons in nondegenerate polar semiconductors is studied when several elastic scattering mechanisms are simultaneously active also. The simple model of the band structure, and the displaced Maxwellian distribution function are used. Analytical expressions for drift mobility are given for  $B = 0$  and the quantum limit, and are compared with the results of other techniques where possible. The numerical calculations show that whenever magnetophonon oscillations are seen in the ohmic regime, maxima occur near the resonance magnetic fields for all lattice temperature and strengths of scattering mechanisms which compete with the optical phonon scattering. This is in contrast with typical experimental findings, in which minima usually (but not always) appear near the resonance fields for ohmic, longitudinal, conditions. The explanation of the minima must therefore be sought in the use of a distribution function in which carrier-carrier scattering is less important.

**TN615. WR15 thermal noise standard,** W. C. Daywitt, W. J. Foote, and E. Campbell, Nat. Bur. Stand. (U.S.), Tech. Note 615, 154 pages (Mar. 1972).

Key words: Error analysis; millimeter wave; noise; Nyquist's theorem; thermal noise standard.

This note describes the design and construction of a WR15 thermal noise power standard. The standard is designed to operate around the Silver Point Temperature (963.19 °C) with a noise temperature output accurate to approximately  $\pm 2$  K.

Complete details of the theory, design, construction, and performance tests are given.

**TN616. Frequency standards and clocks: A tutorial introduction,** H. Hellwig, Nat. Bur. Stand. (U.S.), Tech. Note 616, 69 pages (Apr. 1972).

Key words: Cesium beam; clocks (atomic); crystal oscillator; frequency accuracy; frequency stability; frequency standards; hydrogen maser; quartz crystal; rubidium gas cell; timekeeping.

The topic of frequency standards and clocks is treated in a tutorial and nonmathematical way. The concepts of time, frequency, frequency stability, and accuracy are introduced. The general physical principles and design features of frequency standards and clocks are described. The design, performance, and limitations of quartz crystal oscillators and atomic devices (cesium, hydrogen, rubidium) are discussed in detail and critically compared for laboratory devices as well as for devices intended for field usage.

**TN617. Thermophysical properties of parahydrogen from the freezing liquid line to 5000 R for pressures to 10,000 psia,** R. D. McCarty and L. A. Weber, Nat. Bur. Stand. (U.S.), Tech. Note 617, 169 pages (Apr. 1972).

Key words: Density; dielectric constant; enthalpy; entropy; equation of state; fixed points; heat transfer coefficients; hydrogen; index of refraction; Joule-Thomson; latent heat; melting point; Prandtl number; specific heat; speed of sound; surface tension; thermal conductivity; thermal diffusivity; vapor pressure; viscosity; volume.

Tables of thermophysical properties of para hydrogen are presented for temperatures from the melting line to 5000 R for pressures from 1 to 10,000 psia. The tables include entropy, enthalpy, internal energy, density, volume, speed of sound, specific heat, thermal conductivity, viscosity, thermal diffusivity, Prandtl number and the dielectric constant for 65 isobars. Also included in the isobaric tables are quantities of special utility in heat transfer and thermodynamic calculations:  $(\partial P/\partial V)_T$ ,  $(\partial P/\partial T)_V$ ,  $V(\partial H/\partial V)_P$ ,  $V(\partial P/\partial U)_V$ ,  $-V(\partial P/\partial V)_T$ ,  $1/V(\partial V/\partial T)_P$ .

In addition to the isobaric tables, tables for the saturated vapor and liquid are given which include all of the above properties, plus the surface tension. Tables for the P-T of the freezing liquid, index of refraction and the derived Joule-Thomson inversion curve are also presented.

**TN618. WR15 microwave calorimeter and bolometer unit,** M. E. Harvey, Nat. Bur. Stand. (U.S.), Tech. Note 618, 41 pages (May 1972).

Key words: Calorimeter; microwave; power; standard.

A microwave calorimeter which serves as the National Bureau of Standards (NBS) standard for power measurements in the frequency range 50 to 75 GHz has been completed and evaluated recently. Included here are descriptions of the principal changes in the calorimeter and bolometer unit from the WR28 models which are of similar design. Also included are construction details, accessory equipment, operation procedure, and error analysis. An improved thermal isolating waveguide section and calorimeter flange are features of this calorimeter.

A careful error analysis permits the determination of the effective efficiency of a standard bolometer unit to estimated limits of systematic uncertainty of  $\pm 0.23\%$ . The estimated  $3\sigma$  limit of random uncertainty is 0.05%.

**TN619. Millimeter attenuation and reflection coefficient measurement system,** B. C. Yates and W. Larson, Nat. Bur. Stand. (U.S.), Tech. Note 619, 175 pages (July 1972).

Key words: Attenuation; measurement system; millimeter; reflection coefficient, VSWR.

This paper presents the details to implement a WR 15 attenuation and reflection coefficient magnitude measurement system. A discussion of precision and of systematic error is given along with equations for estimating limits of the error. Machine drawings are provided to fabricate the waveguide standards and necessary hardware not commercially available.

**TN621. Liquid-vapor equilibrium in the binary systems of He<sup>4</sup> and He<sup>3</sup> with nD<sub>2</sub> and nH<sub>2</sub>,** M. J. Hiza, Nat. Bur. Stand. (U.S.), Tech. Note 621, 66 pages (July 1972).

Key words: Binary systems; gas solubility; He<sup>4</sup>-nD<sub>2</sub>; He<sup>3</sup>-nD<sub>2</sub>; He<sup>4</sup>-nH<sub>2</sub>; He<sup>3</sup>-nH<sub>2</sub>; liquid-vapor equilibrium; nD<sub>2</sub> vapor pressure; nH<sub>2</sub> vapor pressure.

Experimental data are reported for the equilibrium liquid and vapor phase compositions of the He<sup>4</sup>-nD<sub>2</sub> and He<sup>3</sup>-nD<sub>2</sub> systems from 20 to 30 K and the He<sup>4</sup>-nH<sub>2</sub> and He<sup>3</sup>-nH<sub>2</sub> systems from 20 to 28 K. The maximum experimental pressures were 20 and 16 atm (2.0 and 1.6 MN/m<sup>2</sup>) for the He<sup>4</sup> and He<sup>3</sup> systems, respectively. In addition, vapor pressures were measured from 20 to 34 K for nD<sub>2</sub> and from 20 to 30 K for nH<sub>2</sub>.

Values of Henry's constants, enhancement factors, K-values, and heats of solution were derived from the experimental data for each system. The derived properties are compared with those derived from previous data for the He<sup>4</sup>-nH<sub>2</sub>, He<sup>4</sup>-pH<sub>2</sub>, and He<sup>3</sup>-nH<sub>2</sub> systems.

**TN622. Thermophysical properties of helium-4 from 4 to 3000 R with pressures to 15,000 psia, R. D. McCarty, Nat. Bur. Stand. (U.S.), Tech. Note 622, 141 pages (Sept. 1972).**

**Key words:** Density; dielectric constant; enthalpy; entropy; equation of state; fixed points; heat transfer coefficients; helium 4; index of refraction; Joule-Thomson coefficient; lambda line; latent heat; melting point; Prandtl number; specific heats; speed of sound; surface tension; thermal conductivity; thermal diffusivity; vapor pressure; viscosity; volume.

Tables of thermophysical properties of helium 4 are presented for temperatures from 4 to 3000 Rankine for pressures to 15,000 psia. The tables include entropy, enthalpy, internal energy, density, volume, speed of sound, specific heat, thermal conductivity, viscosity, thermal diffusivity, Prandtl number and the dielectric constant for 74 isobars. Also included in the isobaric tables are quantities of special utility in heat transfer calculations:  $(\partial P/\partial V)_T$ ,  $(\partial P/\partial T)_P$ ,  $V(\partial H/\partial V)_P$ ,  $V(\partial P/\partial U)_V$ ,  $-V(\partial P/\partial V)_T$ ,  $1/V(\partial V/\partial T)_P$ .

In addition to the isobaric tables, tables for the saturated vapor and liquid are given which include all of the above properties, plus the surface tension. Tables for the  $P\rho T$  of the freezing liquid,  $P\rho T$  of the lambda line, index of refraction and the derived Joule-Thomson inversion curve are also presented.

**TN623. Invariance of the cross ratio applied to microwave network analysis, R. W. Beatty, Nat. Bur. Stand. (U.S.), Tech. Note 623, 23 pages (Sept. 1972).**

**Key words:** Anharmonic ratio; automatic network analyzers; cross ratio; microwave network analysis; reflection coefficient; scattering coefficient.

The historical background and theory is given of the application of the mathematical principle "invariance of the cross ratio" to microwave network analysis. Further developments to improve the accuracy of automatic network analyzers are suggested.

**TN624. An evaluation of several cryogenic turbine flowmeters, J. A. Brennan, R. W. Stokes, D. B. Mann, and C. H. Kneebone, Nat. Bur. Stand. (U.S.), Tech. Note 624, 90 pages (Oct. 1972).**

**Key words:** Cryogenic; flow; liquid nitrogen; mass; mass flowmeters; measurement; turbine flowmeters; volume flowmeters.

The National Bureau of Standards (NBS) and the Compressed Gas Association (CGA) have jointly sponsored a research program on cryogenic flow measurement. A cryogenic flow research facility was constructed and has been used to evaluate cryogenic flowmeters operating on several different principles.

The operation and the accuracy of the flow facility is briefly described. The performance of the flowmeters in liquid nitrogen is described by reporting the precision and bias of the meters before and after an 80-hour stability test and by defining the existence of temperature, pressure, flow rate, subcooling, and time order (wear) dependencies.

Meters were evaluated with flow rates ranging from 20 to 210 gpm (1.3 to 13.2 l/s), pressures ranging from 32 to 112 psia (0.22 to 0.77 MN/m<sup>2</sup>), and with temperatures ranging from 72 to 90 K.

**TN700. COMBO: A general-purpose program for searching, annotating, encoding-decoding, and reformatting data files, R. McClenon and J. Hilsenrath, Nat. Bur. Stand. (U.S.), Tech. Note 700, 68 pages (1972).**

**Key words:** Alphanumeric data files; data retrieval; editing program; file editor; FORTRAN program; general-purpose modular programming; reformatting program; report generator; searching program.

COMBO, a FORTRAN program for searching magnetic tape files, generating reports, and reformatting the file, is described and listed. The program is capable of reading separate card images from a file blocked in physical records and recognizing logical blocks marked by a fixed-field ID. Up to 99 different types of lines, each with its own format, can be recognized by examining a special code or label. The program can be instructed to search for the occurrence of each of certain character strings, using a different list for each type of line and two levels of Boolean logic. Lines can be broken into pieces, using either a fixed-field format or a single separator or flags to define the pieces, and the pieces can be rearranged, with labels or comments optionally inserted between them. Editing, in which specified strings are replaced by other strings, can also be performed. The program can accommodate a variable number of cards of each type per block. It was assembled from general-purpose subroutines of modular design and is substantially machine-independent.

**TN701. Unassigned.**

**TN704. Unassigned.**

**TN705. Tabulation of voluntary national standards, industry standards, international recommendations and certification programs for consumer products, S. J. Chumas, Nat. Bur. Stand. (U.S.), Tech. Note 705, 74 pages (Dec. 1971).**

**Key words:** Certifications programs; consumer products; household products; industry standards; international recommendations; national standards; product standards; standards.

This tabulation is a revision of the Draft Tabulation compiled by the American National Standards Institute and issued in April 1970. The categories and products listed are based on the Consumer Product Safety Index of the National Commission on Product Safety, July 1970. The consumer products listed are mostly those that are used in or around the home. The notable exception is sports and recreational equipment. The major consumer product areas not included are foods, beverages, and drugs.

The tabulation lists 385 product areas and indicates the applicable voluntary national, industrial, and international standards which deal primarily with either safety or performance or both aspects of the product. For some of these areas, there are no applicable standards. Available information on certifications programs is also indicated.

**TN706. Structural performance evaluation of innovative building systems, F. Y. Yokel and N. F. Somes, Nat. Bur. Stand. (U.S.), Tech. Note 706, 16 pages (Aug. 1972).**

**Key words:** Building; connections; housing; neoprene; performance criteria; performance evaluation; performance testing; reinforced concrete; standard tests; structure, testing.

Considerable attention has recently been focused on the development of performance criteria. Performance criteria are presently used in the U.S. by the Building Research Division of the Institute for Applied Technology, National Bureau of Standards, to evaluate innovative building systems.

While building codes and design standards are usually related to specific building materials and design solutions, performance criteria are derived from user requirements and are independent of specific technological solutions.

Many attributes inherent in traditional building systems which are acceptable to the user may not be present in untried innovative systems. The performance criteria therefore address themselves to many aspects of structural performance which are not considered in present codes and design standards.



The successful application of performance criteria depends on the feasibility of evaluating compliance.

Performance can be evaluated by analysis by judgment based on past experience, or by physical simulation. Deterioration with time must be considered, and performance criteria are viewed as minimum requirements which should be met at any time during the service life of a structure. An example is presented where physical testing was used to evaluate the performance of a high-rise housing system.

**TN707. Three-year inspection of nature-tone porcelain enamels on steel, M. A. Baker, Nat. Bur. Stand. (U.S.), Tech. Note 707, 16 pages (Dec. 1971).**

**Key words:** Acid resistance; color; continuity of coating; porcelain enamel; weather resistance.

A weather exposure test on nature-tone porcelain enamels on steel was initiated by the National Bureau of Standards and the Porcelain Enamel Institute in 1966. Laboratory measurements for changes in gloss and color were made after the enamels had been exposed for 0.5, 1 and 3 years at Kure Beach, N.C., Miami, Fla. and Gaithersburg, Md. The average gloss and color retained for all 450 specimens exposed at 3 sites for 3 years were 90.5 and 99.1 respectively. There was a tendency for the enamels exposed at the marine sites to rust around pinhole-type defects. Scanning electron microscope studies of these defects showed a layer of readily corrodible enamel on the bottom of the defects. A high-voltage test for continuity of coating was effective in detecting specimens that were apt to rust during the first year's exposure.

**TN709. An x-ray diffraction method for determining the amount of austenite in an austenite-ferrite mixture, C. J. Bechtoldt, Nat. Bur. Stand. (U.S.), Tech. Note 709, 15 pages (Feb. 1972).**

**Key words:** Austenite; computer; ferrite; phase measurement; quantitative analysis; retained austenite; x-ray diffraction.

A method for determining the relative phase volume of austenite in an austenite-ferrite mixture is described in detail. Results obtained by applying this method to an austenite-ferrite stainless steel composite material are presented. The method can be extended to other multi-phase materials.

**TN710-1. Building research translation: Account of the principles of modular coordination: Industrialization in building, G. Blachère, Nat. Bur. Stand. (U.S.), Tech. Note 710-1, 15 pages (Mar. 1972).**

**Key words:** Conventions; dimensional coordination; industrialized production; modular coordination; tolerance.

This paper is translated from the French original and is published under the Building Research Division/Centre Scientifique et Technique du Bâtiment information exchange program.

Modular coordination is indispensable to the industrialized production of units for assembly in buildings. It must be subject to the limitations which are strictly necessary to achieve this end. A large module must be chosen, the reference for the coordinating dimensions must be fixed, and the tolerance problem solved. This is the theme of the report.

**TN710-2. Building research translation: An investigation of the protection of dwellings from external noise through facade walls, P. Gilbert, Nat. Bur. Stand. (U.S.), Tech. Note 710-2, 26 pages (Mar. 1972).**

**Key words:** Facade; noise; sound insulation; sound pressure level; walls.

This paper is translated from the French original and is published under the Building Research Division/Centre Scientifique et Technique du Bâtiment information exchange program.

An investigation was conducted to determine to what extent the installation of balconies and loggias at various angles of elevation from a noise source could improve the sound insulation of a facade wall. Measurements of the sound pressure level were first carried out on two types of facade, one incorporating traditional window joinery and the other incorporating sealed glazing. Following this, the sound insulation provided by facades fitted with open and closed balconies and loggias (with and without sound absorbent materials applied) was determined and compared with the previous measurements. It was found that for angles of elevation greater than 30°, both the closed balcony and the loggia fitted with absorbent materials appreciably improve the sound insulation, whereas the open balcony does not.

**TN710-3. Building research translation: New regulation on ventilation of dwellings, fixed heating facilities, and flues, A. Chalandon, M. Schumann, and P. Dechartre, Nat. Bur. Stand. (U.S.), Tech. Note 710-3, 46 pages (May 1972).**

**Key words:** Air infiltration and extraction, airtightness; discomfort index; duct system, collective and individual branch; flow rates; noise; pressure-loss-depression; thermal convection; ventilation.

Following studies on the ventilation of dwellings, the results of which have been published in CSTB "Cahiers," the CSTB has proposed certain changes in the regulations governing the ventilation of dwellings. At the same time, in the light of recent statistics on secondary emergency and relief heating, changes in the regulations governing fixed heating installations and flues were proposed. These proposals led to a new revised text of the French regulations, which we publish below, together with a new chapter on "ventilation" from the CSTB Technical Report.

**TN710-4. Building research translation: Thermal comfort requirement adjacent to cold walls—application to glazed opening, J. Anquez and M. Croiset, Nat. Bur. Stand. (U.S.), Tech. Note 710-4, 54 pages (May 1972).**

**Key words:** Curtains, effect of; environmental conditions; glazed openings; human response; thermal comfort requirement.

This paper is translated from the French original and is published under the Building Research Division/Centre Scientifique et Technique du Bâtiment information exchange program.

The thermal comfort of an individual inside a closed room in winter is essentially a function of the temperature of the air with which the human body transfers heat by convection, and also of the temperature of the room's walls with which the human body transfers heat by radiation. The presence of glazed openings (windows) which in winter are generally the coldest walls in a residence room, can thus be a source of discomfort.

The first part of the paper reports research conducted with a view to determining the thermal comfort requirement near to a cold wall. The research led to the definition of the "air-radiation requirement" for a plane surface element parallel to the wall, the requirement being that, at about 1 m from the wall, this temperature must remain above 16 or 17 °C.

The second part of the paper studies ways of satisfying the requirement near to glazed openings in a living room in winter. The solution to the problem will depend on numerous factors: climatic zone, average temperature of the room, position of heat sources, dimensions of the openings, type of glazing (single or double), presence or absence of curtains or screens.

**TN710-5. Building research translation: Use of an air-to-air heat exchanger to recover heat from air exhausted by mechanical ventilation,** P. Garrivier, Nat. Bur. Stand. (U.S.), Tech. Note 710-5, 62 pages (July 1972).

Key words: Exchanger dimensions; frost formation; heat exchanger; heating costs; mechanical systems; pollution; pressure loss; ventilation.

When a building is equipped with a mechanical system which both exhausts and supplies outdoor air, it may be profitable to install a heat exchanger between the two circuits. The CSTB has perfected such an exchanger, which meets the two principal requirements of the problem: good efficiencies and elimination of the polluted air intake. A method of calculating the optimal dimensions of the exchanger has also been devised.

**TN711. Measures for air quality, annual report—FY 1971,** J. R. McNesby and R. Byerly, Jr., Nat. Bur. Stand. (U.S.), Tech. Note 711, 77 pages (Jan. 1972).

Key words: Air pollution; carbon monoxide; hydrocarbons; nitrogen oxide; ozone; particulates; standard reference materials; sulfur dioxide.

A compilation of reports covering the air pollution related projects at NBS during FY 1971. There are 23 projects in all, and they cover many areas of air pollution measurement. A table of contents lists descriptive project titles.

**TN712. Manual and computerized footprint identification,** J. H. Wegstein, Nat. Bur. Stand. (U.S.), Tech. Note 712, 13 pages (Feb. 1972).

Key words: Computerized-footprint-identification; footprint; pattern recognition.

Part 1 describes a manual footprint classification system that utilizes the ridge patterns adjacent to the toes on the sole of the right foot. This system is an extension of the FBI footprint classification system. Part 2 describes a method of coding minute details of these prints for storage in a computerized file. The computer can then search a similarly coded unknown print against this file and identify the most likely matching prints from the file.

**TN713. Electromagnetic multipole transitions in the recoupling picture, or, electron scattering without curls,** J. S. O'Connell, Nat. Bur. Stand. (U.S.), Tech. Note 713, 20 pages (Feb. 1972).

Key words: Electric transitions; electromagnetic operators; electron scattering; magnetic transitions; multipoles; recoupling.

The formation of the multipole operators from the fundamental charge, current, and moment operators of electron-nucleus scattering is carried through as an angular momentum recoupling problem rather than the usual vector algebra derivation. This point of view allows the electric and magnetic transition operators to be obtained in a simple and intuitive manner. The single particle reduced matrix elements of the charge, current, and moment operators are then calculated in the  $j$ - $j$  coupling scheme using a flow chart technique developed by Danos.

**TN714. Reactor Radiation Division: Annual progress report for the period ending October 31, 1971,** R. S. Carter, Editor, Nat. Bur. Stand. (U.S.), Tech. Note 714, 108 pages (Mar. 1972).

Key words: Crystal structure; diffraction; isotope, molecular structure; neutron; nuclear reactor; radiation.

The report is the annual progress report of the Reactor Radiation Division for the period October 1, 1970 to October 1, 1971.

It summarizes the activities of the large number of users outside the Division as well as the work in the Division.

**TN715. Tabulation of published data on electron devices of the U.S.S.R. through December 1971,** C. P. Marsden, Nat. Bur. Stand. (U.S.), Tech. Note 715, 108 pages (June 1972).

Key words: Electron devices; electron tubes; semiconductor; U.S.S.R.

This tabulation includes published data on U.S.S.R. electron devices as collected from publications, mostly handbooks, published by the various ministries and institutes of the U.S.S.R. Information is given on all active devices ranging from receiving to microwave devices, semiconductor devices, and miscellaneous devices such as photographic flash tubes and thermistors. Supersedes NBS TN526.

**TN716. The ideal Lovibond color system for CIE standard illuminants A and C shown in three colorimetric systems,** G. W. Haupt, J. C. Schleter, and K. L. Eckerle, Nat. Bur. Stand. (U.S.), Tech. Note 716, 115 pages (Apr. 1972).

Key words: Chromaticity, Lovibond; CIE and Lovibond; colorimetry, Lovibond; color, Lovibond; glass color standards; Lovibond and CIE.

Tables are given which list luminous internal transmittances, luminous transmittances, and chromaticity coordinates of the ideal Lovibond color system for CIE standard illuminants A and C according to (1) the CIE 1931 (x,y)-system, (2) the CIE 1960 uniform-chromaticity-scale (UCS) (u,v)-system, and (3) the CIE 1964 ( $U^*$ ,  $V^*$ ,  $W^*$ )-system. Chromaticity diagrams for the (x,y)- and (u,v)-systems are shown together with horizontal and vertical cross-sections of the ( $U^*$ ,  $V^*$ ,  $W^*$ ) color solid for the entire ideal Lovibond color system produced by single-color units and two-color combinations of units for each illuminant. In addition, chromaticity diagrams and cross-sections are shown indicating the single color units of red, yellow, and blue for each CIE system and illuminant.

**TN717. Methods of measurement for semiconductor materials, process control, and devices, quarterly report, July 1 to September 30, 1971,** W. M. Bullis, Editor, Nat. Bur. Stand. (U.S.), Tech. Note 717, 52 pages (Apr. 1972).

Key words: Alpha-particle detectors; aluminum wire; base transit time; carrier lifetime; die attachment; electrical properties; epitaxial silicon; gamma-ray detectors; germanium; gold-doped silicon; infrared response; methods of measurement; microelectronics; microwave diodes; nuclear radiation detectors; probe techniques (a-c); resistivity; semiconductor devices; semiconductor materials; semiconductor process control; silicon; thermal resistance; thermographic measurements; ultrasonic bonder; wire bonds.

This quarterly progress report, thirteenth of a series, describes NBS activities directed toward the development of methods of measurement for semiconductor materials, process control, and devices. Significant accomplishments during this reporting period included the disclosure of substantial differences in measurements of transistor delay time, a device characteristic frequently used as a screen in radiation hardness assurance tests, as measured with two different instruments; successful application of the infrared response technique to the study of radiation-damaged, lithium-drifted silicon detectors; and identification of a condition that minimizes wire flexure and reduces the failure rate of transistors under slow thermal cycling conditions. Work is continuing on measurement of resistivity of semiconductor crystals; study of gold-doped silicon; specification of germanium for gamma-ray detectors; evaluation of wire bonds and die attachment; measurement of thermal properties of semiconductor



devices; noise properties of microwave diodes; and characterization of silicon nuclear radiation detectors. Supplementary data concerning staff, standards committee activities, technical services, and publications are included as appendixes.

**TN718. Magnetic recording of acoustic data on audiofrequency tape recorders**, E. D. Burnett, E. L. R. Corliss, and R. D. Berendt, Nat. Bur. Stand. (U.S.), Tech. Note 718, 29 pages (Apr. 1972).

**Key words:** Acoustic measurements; calibrated tape recordings; data acquisition; magnetic recording; psychoacoustic data; recordings in the field; tape recording.

This Technical Note discusses the application of magnetic tape recording to storage and analysis of data obtained in the course of acoustic measurements. In general, the most suitable machines are those designed primarily for recording studios. Advantages in signal-to-noise ratios and extended linear range can be realized by careful choice of recording medium, adjustment of the equipment to optimum performance, and proper care in monitoring the recording process. General instructions for realizing these advantages are given. Particular emphasis is given to the procedures for making well-calibrated recordings in the field, for analysis of noise problems.

**TN719. A simple correction procedure for quantitative electron probe microanalysis**, K. F. J. Heinrich, R. L. Myklebust, H. Yakowitz, and S. D. Rasberry, Nat. Bur. Stand. (U.S.), Tech. Note 719, 49 pages (May 1972).

**Key words:** Absorption; atomic number; chemical elements; computation procedure; data reduction; electron probe microanalysis; fluorescence; time-sharing; x-ray analysis.

A calculation technique for data reduction in quantitative electron probe microanalysis is described. This technique is embodied in a computer program, called MULTI8, written in FORTRAN IV for batch processing. Six chemical elements may be determined simultaneously without redimensioning the program. The relative x-ray intensity data are corrected for atomic number, absorption and secondary fluorescence due to the characteristic lines. Options for calculating the mass fraction of one chemical element by difference or by stoichiometry are available in the program. Supersedes and extends NBS TN521.

**TN720. A simple hydraulic sinusoidal pressure calibrator**, J. S. Hilten, P. S. Lederer, and J. Sethian, Nat. Bur. Stand. (U.S.), Tech. Note 720, 27 pages (Apr. 1972).

**Key words:** Calibrator; dynamic; hydraulic; InterAgency Transducer Project; pressure transducer; sinusoidal pressure.

This paper describes a simple, accurate device for the sinusoidal calibration of pressure transducers. Calibration is achieved by vibrating a liquid tube on an electrodynamic shaker (vibration generator); the pressure transducer mounted at the base of the tube senses the sinusoidally varying pressure in the tube. The frequency range is 15 Hz to 2000 Hz with a maximum obtainable amplitude of 19.5 psi (134 kN/m<sup>2</sup>) peak to peak. The transducer can easily be calibrated statically in the same device, thus permitting precise correlation between static and dynamic calibrations. Agreement between static and dynamic calibrations to within 0.1% has been achieved.

**TN721. NBS Special Foreign Currency Program in Israel 1970-71**, H. S. Peiser and M. Klein, Nat. Bur. Stand. (U.S.), Tech. Note 721, 175 pages (Apr. 1972).

**Key words:** Binational research cooperation; international scientific cooperation; Israel science and technology; physical

science research administration; PL-480 programs; research planning; scientific research abstracts.

An overview is given of grants awarded by the National Bureau of Standards under the Special Foreign Currency Program in Israel authorized by Public Law 480 and its amendments. Each grant is identified by title, principal investigator, institution in Israel, NBS monitor working in close technical touch with the project in Israel, and the monitor's organizational unit within NBS. The relevant work is then described briefly under the three headings "Summary of Description of Project Goals," "Results and Implications to Date" and "List of Publications that Resulted from the Project." To demonstrate the wide use of such grants over the entire Program Structure of NBS, the grant descriptions are ordered by the elements of that Program Structure. Editorial comment on the significance and purpose of the NBS/PL 480 grant program is confined to a Foreword and Introduction. The editors judge this grant program to have had a high benefit to cost ratio from the viewpoint of NBS.

**TN722. Tensile creep of boron epoxy and boron epoxy-reinforced 7075-T6 aluminum alloy**, D. J. Chwirut, Nat. Bur. Stand. (U.S.), Tech. Note 722, 60 pages (May 1972).

**Key words:** Aluminum alloy; boron/epoxy; composite materials; creep; elastic follow-up technique; sandwich specimen.

Tensile creep tests were performed on twelve specimens of 0° unidirectional boron/epoxy and on twenty-four specimens of 7075-T6 aluminum alloy reinforced with 0° unidirectional boron/epoxy. An analytical procedure for predicting the creep properties of composite-reinforced metals is presented. Agreement between calculated and experimental creep curves varies with test temperature. These discrepancies between experiment and analysis are probably not due to an error in the analysis itself, but rather to uncertainty in the residual stresses in the specimens.

**TN723. A laser technique for investigating the effects of thermal transients on pressure transducer performance characteristics**, P. S. Lederer and J. S. Hilten, Nat. Bur. Stand. (U.S.), Tech. Note 723, 43 pages (May 1972).

**Key words:** Laser; performance characteristic; pressure transducer; temperature effects; test method; thermal transient.

A simple and repeatable testing technique was developed which makes it practical to obtain information on the zero shift and change in sensitivity of a pressure transducer while it is subjected to a thermal transient generated by a mechanically chopped cw laser beam. Several commercial, flush diaphragm, pressure transducers with ranges from up to 50 psi ( $3.45 \times 10^5$  N/m<sup>2</sup>) were tested and showed zero shifts and changes in sensitivity of the order of 20% FS due to thermal transients with power densities up to 100 K W/m<sup>2</sup>. The transducer under test can be pressure cycled while it is irradiated. In this way, zero shifts and sensitivity changes may be directly displayed in a procedure which requires a testing time of only about one minute.

**TN724. Properties of selected superconductive materials**, B. W. Roberts, Nat. Bur. Stand. (U.S.), Tech. Note 724, 100 pages (June 1972).

**Key words:** Bibliography; compilation of data; composition; critical field; critical temperature; crystallographic data; low temperature; superconductivity.

This is a noncritical compilation of data on superconductive materials with the exception of data on the elements that has been extracted from a portion of the literature published up to



early 1971. The properties concerned are composition, critical temperature, critical magnetic fields, crystallographic data, and the lowest temperature tested for materials specifically explored for superconductivity. The compilation also includes, bibliography, general reference review articles and a special tabulation of high magnetic field superconductors. Supersedes and extends NBS TN482.

**TN725. A neutron moments computer code, moment I, C. M. Eisenhauer, G. L. Simmons, and L. V. Spencer, Nat. Bur. Stand. (U.S.), Tech. Note 725, 38 pages (May 1972).**

**Key words:** Carbon; computer code; gauss quadrature; moments; neutron transport; shielding.

In this paper we discuss a computer code for generating spatial-angular moments of neutron flux in an infinite medium. The equation for the flux moments is given and the techniques used for the solution are discussed. The structure of the computer code and of the main subroutines is also discussed. Details of the input and output data are given and the printout from a sample problem is included.

**TN726. Testing and fabrication of wire-bond electrical connections—a comprehensive survey, H. A. Schafft, Nat. Bur. Stand. (U.S.), Tech. Note 726, 140 pages (Sept. 1972).**

**Key words:** Bonding; degradation (wire bond); discrete devices; electrical interconnection; fabrication (wire bond); failure (wire bond); hybrid circuits; integrated circuits; microelectronics; reliability; semiconductor devices; survey (wire bond); testing (wire bond); thermocompression bonding; ultrasonic bonding; wire bond.

The fabrication and testing of wire-bond electrical connections used in integrated circuits, hybrid circuits, and low-power discrete semiconductor devices are surveyed comprehensively. The survey is generally restricted to wire-bond electrical connections where the wire diameter is less than 2 mils and where the wire is bonded either by thermocompressive or ultrasonic means. Under the general heading of fabrication, the essential features of the thermocompression and ultrasonic bonding processes, the fabrication procedures, and the characteristics of the constituent materials of the wire bond pertinent to high reliability are surveyed. Also included is a review of the interaction of gold and aluminum as one of the primary failure mechanisms in wire bonds. Both new and old test methods are surveyed with emphasis on their capabilities and limitations. In particular, the following test methods are discussed: visual inspection; pull, shear, air blast, push, ultrasonic stress, centrifuge, mechanical shock, variable frequency vibration, vibration fatigue, short-duration stress pulse, temperature cycling, thermal shock, bond interface resistance, and electrical continuity tests; noise measurement; and ultrasonic bond monitoring. Analyses of some of the methods with regard to the stress that the test imposes on the wire bond have been made and the results are used in discussing the relevant methods.

**TN727. Methods of measurement for semiconductor materials, process control, and devices. Quarterly report October 1 to December 31, 1971, W. M. Bullis, Editor, Nat. Bur. Stand. (U.S.), Tech. Note 727, 79 pages (June 1972).**

**Key words:** Alpha-particle detectors; aluminum wire; base transit time; carrier lifetime; die attachment; electrical properties; epitaxial silicon; gamma-ray detectors; germanium; gold-doped silicon; infrared response; methods of measurement; microelectronics; microwave diodes; nuclear radiation detectors; probe techniques (a-c); resistivity; semiconductor devices; semiconductor materials; semiconductor process control; silicon; thermal resistance; thermographic measurements; ultrasonic bonding; wire bonds.

This quarterly progress report, fourteenth of a series, describes NBS activities directed toward the development of methods of measurement for semiconductor materials, process control, and devices. Significant accomplishments during this reporting period included the determination of the reasons for substantial differences in measurements of transistor delay time, a device characteristic frequently used as a screen in radiation hardness assurance tests, as measured with different instruments or with the same instrument at different frequencies; identification of an energy level model for gold-doped silicon that yields a calculated dependence of resistivity on gold concentration that agrees very well with experimental measurements on *p*-type gold-doped silicon; and finding of evidence that it does not appear to be necessary for an ultrasonic bonding tool to grip the wire and move it across the substrate metallization to make the bond. Work is continuing on measurement of resistivity of semiconductor crystals; study of gold-doped silicon; development of the infrared response technique; evaluation of wire bonds and die attachment; measurement of thermal properties of semiconductor devices, delay time and related carrier transport properties in junction devices, and noise properties of microwave diodes; and characterization of silicon nuclear radiation detectors. Supplementary data concerning staff, standards committee activities, technical services, and publications are included as appendixes.

**TN728. Torsional instabilities in composite and composite-reinforced aluminum-alloy thin-walled cylinders, D. E. Marlowe, Nat. Bur. Stand. (U.S.), Tech. Note 728, 77 pages (June 1972).**

**Key words:** Aircraft structures; boron/epoxy; composite materials; reinforced aluminum; stability; thin shells; torsion buckling.

The elastic buckling strength has been determined for thin-walled aluminum-alloy tubes fabricated with and without unidirectional boron/epoxy and glass/epoxy composite materials applied as reinforcement to their outer surfaces. Three boron/epoxy ply orientations were investigated. The results of these tests have been compared with the buckling strengths predicted by two analytical techniques. It was found that reinforcement of the metal tubes with an equal thickness of the composite material increased the buckling strength about threefold. The effect on buckling strength of the ply angles investigated is small when compared with the overall effect of adding the reinforcement. The analyses have approximately the same degree of accuracy as that generally attributed to Donnell's treatment of isotropic tubes.

**TN729. Design, construction, and testing of a new high accuracy spectrophotometer, K. D. Mielenz and K. L. Eckerle, Nat. Bur. Stand. (U.S.), Tech. Note 729, 60 pages (June 1972).**

**Key words:** Beam non-uniformity; circular entrance and exit apertures; high accuracy spectrophotometer; linearity; parabolic mirrors; stray radiant energy; transmittance.

A new spectrophotometer is described which has an accuracy of approximately 0.0001 transmittance units. The spectrophotometer utilizes a collimated beam in the sample area. This is accomplished by means of off-axis parabolic mirrors in the monochromator and sample compartment. Also, circular holes are used as entrance and exit apertures in the monochromator. All components of this spectrophotometer were chosen to achieve maximum accuracy. The result of this work is a "state of the art" instrument. The instrument was tested to evaluate its performance. Systematic errors such as detector non-linearity, stray radiant energy, and beam non-uniformity are measured. A correction for non-linearity of the photomultiplier and electronics is applied.



**TN730. Manual and automated fingerprint registration, J. H. Wegstein, Nat. Bur. Stand. (U.S.), Tech. Note 730, 26 pages (June 1972).**

**Key words:** Computerized-fingerprint-identification; fingerprint; pattern-recognition.

A method is described for manually positioning a fingerprint so that manually read minutiae data can be searched by computer against a file of fingerprint data that has been previously read by machine. A procedure is also described whereby a computer can utilize machine-read ridge-direction data in manipulating minutiae data to effect a registration of the fingerprint prior to filing its minutiae data.

**TN731. Calibration of secondary standard magnetic tape cassettes (computer amplitude reference) Phase I, S. B. Geller and P. A. Mantek, Nat. Bur. Stand. (U.S.), Tech. Note 731, 60 pages (July 1972).**

**Key words:** Cassette tapes; cassette transport; computer amplitude reference; magnetic tape cassette; secondary standard; standard reference material; unrecorded references.

This Technical Note discusses a method for developing and maintaining a reference system which will produce NBS Secondary Standard Magnetic Tape Cassettes (Computer Amplitude Reference). It describes both centerline tape search procedures and an interim signal amplitude measurement system for the reference magnetic tape cassette candidates. The results of the initial experiments with cassette tapes and transports are given.

**TN732. A computer terminal network for transparent stimulation of the user of an on-line retrieval system, S. Treu, Nat. Bur. Stand. (U.S.), Tech. Note 732, 39 pages (July 1972).**

**Key words:** Computer terminal network; human characteristics; interactive information retrieval; man-computer interface; transparent stimulation; unobtrusive monitoring.

A computer terminal network to enable "transparent stimulation" of the user of an on-line retrieval system has been designed, implemented, and pilot tested. Its basic purpose is to provide a suitable and effective framework and methodology for experimental identification/validation of those human characteristics which should be recognized/reinforced in man-computer interface design. The rationale behind the transparent stimulation approach is presented and the methodology employed for such real-time, unobtrusive scanning and manipulation of the man-computer dialogue is described. A general overview of the hardware and software features of the implemented stimulation network is included.

**TN733. Methods of measurement for semiconductor materials, process control, and devices, quarterly report January 1 to March 31, 1972, W. M. Bullis, Editor, Nat. Bur. Stand. (U.S.), Tech. Note 733, 59 pages (Sept. 1972).**

**Key words:** Aluminum wire; base transit time; carrier lifetime; die attachment; electrical properties; epitaxial silicon; gamma-ray detectors; germanium; gold-doped silicon; infrared response; methods of measurement; microelectronics; microwave diodes; nuclear radiation detectors; probe techniques (a-c); resistivity; ribbon wire bonding; semiconductor devices; semiconductor materials; semiconductor process control; silicon; thermal resistance; thermographic measurements; ultrasonic bonding; wire bonds.

This quarterly progress report, fifteenth of a series, describes NBS activities directed toward the development of methods of measurement for semiconductor materials, process control, and devices. Significant accomplishments during this reporting

period include development of a procedure to correct for the substantial differences of transistor delay time, a device characteristic frequently used as a screen in radiation hardness assurance tests, as measured with different instruments or with the same instrument at different frequencies; association of infrared response spectra of poor quality germanium gamma-ray detectors with spectra of detectors fabricated from portions of a good crystal that had been degraded in known ways; and confirmation of the excellent quality and cosmetic appearance of ultrasonic bonds made with aluminum ribbon wire. Work is continuing on measurement of resistivity of semiconductor crystals; study of gold-doped silicon; development of the infrared response technique; evaluation of wire bonds and die attachment; and measurement of thermal properties of semiconductor devices, delay time and related carrier transport properties in junction devices, and noise properties of microwave diodes. Supplementary data concerning staff, standards committee activities, technical services, and publications are included as appendices.

**TN734. OMNITAB II. Segmentation structure for the SCOPE operating system, S. T. Peavy and R. N. Varner, Nat. Bur. Stand. (U.S.), Tech. Note 734, 25 pages (June 1972).**

**Key words:** ANSI FORTRAN; general-purpose computer program; implementation of OMNITAB II; links; OMNITAB II; overlay procedures; SCOPE operating system; segmentation.

OMNITAB II is an interpretive system developed and maintained by the National Bureau of Standards to enable scientists to use a large computer easily, effectively and accurately for numerical, statistical and data analysis without prior computer experience. The system is as machine independent as possible, making implementation relatively easy. Since OMNITAB II has a large memory requirement, segmentation and overlay are virtually essential.

Overlay procedures are dependent upon the operating system of the computer. Changes are necessary to the OMNITAB II program when the overlay procedure requires specific overlay CALL statements to external procedures in other overlay links. This Technical Note describes a method of segmentation and overlay for a particular operating system (CDC-6000 series). The method can readily be adapted to other operating systems with modifications to the control statements.

**TN735. The effects of magnetic fields on magnetic storage media used in computers, S. B. Geller, Nat. Bur. Stand. (U.S.), Tech. Note 735, 35 pages (July 1972).**

**Key words:** Erasure, magnetic media; erasure, permanent magnet; erasure, shielding against; erasure, signal loss due to; magnet fields, erasure with; magnetic media, computer; magnetic media, information damage; permanent magnet, erasure with; permanent magnets; shielding.

Experiments have been performed with different types of magnets to determine their effects on the information stored on magnetic storage media. The test results that were obtained with recorded computer tapes are discussed and guidelines are suggested to computer installation managers for protecting their recorded tapes, disks and drums against unwarranted erasure by magnetic fields. The effects of other forms of energy on recorded magnetic media are briefly considered.

**TN736. Carrier lifetime measurement by the photoconductive decay method, R. L. Mattis and A. J. Baroody, Jr., Nat. Bur. Stand. (U.S.), Tech. Note 736, 52 pages (Sept. 1972).**

**Key words:** Carrier lifetime; germanium; photoconductive decay; silicon.

The photoconductive decay (PCD) method of carrier lifetime measurement is discussed with emphasis on experimental and analytical work done at NBS. The relationship between photoconductive decay time  $\tau_{PCD}$ , bulk decay time  $\tau_B$ , and lifetime is described briefly and the PCD method is summarized. The determination of  $\tau_B$  from  $\tau_{PCD}$  and the influence of higher modes of recombination are discussed.

Experimental data, supported by theoretical considerations, are presented to demonstrate the dependence of  $\tau_{PCD}$  on excess carrier density, the type of light source, specimen homogeneity, filter thickness, and temperature. The dependences of  $\tau_{PCD}$  on excess carrier density and temperature are consequences of the statistics of the recombination process. Measurements made with chopped light excitation are shown to be less in error due to higher modes of recombination than are measurements made with pulsed light excitation. The presence of inhomogeneities is verified in two crystals. Use of a filter is also shown to reduce the influence of higher modes. An unexpected reduction in  $\tau_{PCD}$  with increasing filter thickness is shown to be caused by an inhomogeneity.

Other experimental conditions are discussed as they affect the measurement of  $\tau_{PCD}$ . It is shown that the light turnoff must be sufficiently fast and the series resistance sufficiently large that they do not interfere with the measurement. Equations are developed whereby the specimen current and illumination pattern can be chosen such that carrier sweep-out at the ends of the specimen and ohmic heating are avoided. The end contacts must be sufficiently ohmic that excessive contact resistance does not interfere with the measurement.

Trapping is defined and the means for identifying it are discussed briefly. The PCD method is inappropriate for determining minority carrier lifetime when trapping is present or under other circumstances when the hole and electron lifetimes are unequal.

**TN737. Interior/exterior noise levels of over-the-road trucks: report of tests,** W. A. Leasure, Jr., T. L. Quindry, D. E. Mathews, and J. M. Heinen, Nat. Bur. Stand. (U.S.), Tech. Note 737, 317 pages (Sept. 1972).

Key words: Acoustics; noise measurement; noise (sound); truck noise (exterior); truck noise (interior); trucks.

This report presents the results of interior and exterior noise measurements which were made on a representative sample of fifteen over-the-road trucks under various operational modes. In-cab measurements were made six inches from the right and left ears of the driver with windows open and closed. Simultaneous exterior measurements were made utilizing a six-microphone array. Graphic histories of A-weighted sound level versus time are presented for all test conditions and microphone locations. The National Bureau of Standards made the field measurements and tabulated the data; however, interpretation of the results is the responsibility of the Department of Transportation and the American Trucking Associations—the joint sponsors of the study. These data supplement the limited in-cab data available in the public domain and will form part of public Docket No. MC-22 Advanced Notice of Proposed Rule Making concerning vehicle interior noise levels which was issued by the Bureau of Motor Carrier Safety, Department of Transportation, in response to Federal Regulations concerning occupational noise exposure.

**TN738. Subroutine for the calculation of CODEN check characters,** D. Garvin, Nat. Bur. Stand. (U.S.), Tech. Note 738, 12 pages (Sept. 1972).

Key words: Check characters; CODEN; computer program; journal abbreviations.

A FORTRAN subroutine is described that computes the check character for an ASTM CODEN for Journal Titles. This routine, written for input in Hollerith characters, is adaptable to other coding schemes. A listing of the routine is provided.

**TN739. A universal dropout tester for magnetic storage media,** S. B. Geller, Nat. Bur. Stand. (U.S.), Tech. Note 739, 32 pages (Sept. 1972).

Key words: Dropouts, cassette tapes; dropouts, computer magnetic tapes; dropouts, instrumentation magnetic tapes; dropouts, measurement system; magnetic storage media; signal amplitude, dropouts.

This Technical Note describes a signal dropout detection and counting system which was designed to make measurements on 1/2 inch magnetic computer tape, magnetic instrumentation tapes and magnetic cassette tapes as required by existing and potential Federal Specifications. The calibration and operational procedures for the system are described in detail.

**TN742. United States and Canadian fabric flammability standards,** R. G. Katz, Nat. Bur. Stand. (U.S.), Tech. Note 742, 59 pages (Oct. 1972).

Key words: Blankets; Canada; carpets; clothing; fabric flammability testing; fabrics; Flammable Fabrics Act; Hazardous Products Act; mattresses; sleepwear; standards; United States.

Current fabric flammability standards of the United States and Canada are described. The 1967 amendment to the Flammable Fabrics Act of 1953 gave impetus to basic and applied research in the United States and to the development of new test methods and standards for fabric products. Commercial Standard 191-53, the 45-degree angle test, applies to most clothing items, but a new stringent vertical test was developed for children's sleepwear. A small flame source, i.e., a standard methenamine tablet, is used to test carpets and rugs, while a smoldering cigarette is the ignition source for a mattress standard. The test methods attempt to simulate actual conditions.

In 1970, Canada amended the Hazardous Products Act of 1969 to (a) ban from sale those products already declared dangerously flammable by the United States, and (b) ban from sale some berets and sweatshirts that did not meet the 45-degree angle test. Later amendments (1971) deleted the 1970 amendments and established a basic minimum flammability standard covering all textile products for consumer use. A more stringent standard was established for children's sleepwear and bedding (excluding mattresses, mattress pads and pillows) that use the same 45-degree angle test but with a time of flame spread of 7 seconds or less.

**TN743. Methods of measurement for semiconductor materials, process control, and devices, quarterly report April 1 to June 30, 1972,** W. M. Bullis, Editor, Nat. Bur. Stand. (U.S.), Tech. Note 743, 57 pages (Dec. 1972).

Key words: Aluminum wire; base transit time; carrier lifetime; die attachment; electrical properties; epitaxial silicon; gamma-ray detectors; generation centers; germanium; gold-doped silicon; infrared response; methods of measurement; microelectronics; microwave diodes; nuclear radiation detectors; probe techniques (a-c); recombination centers; resistivity; ribbon-wire bonding; semiconductor devices; semiconductor materials; semiconductor process control; silicon; thermal resistance; trapping centers; ultrasonic bonding; wire bonds.

This quarterly progress report, sixteenth of a series, describes NBS activities directed toward the development of methods of measurement for semiconductor materials, process control, and



devices. Significant accomplishments during this reporting period include verification of the applicability of resolution of forces in interpreting pull test measurements on unannealed wire bonds on single-level substrates, completion of the feasibility study of ribbon-wire bonding with the important finding that ribbon-wire bonds can be made with a wider range of bonding parameters than round-wire bonds of the same strength, and development of test procedures in preparation for studies of high-frequency measurements of transistors on the wafer by means of probes. Work is continuing on measurement of resistivity of semiconductor crystals; study of gold-doped silicon; development of the infrared response technique; evaluation of wire bonds and die attachment; and measurement of thermal properties of semiconductor devices, delay time and related carrier transport properties in junction devices, and noise properties of microwave diodes. New work has been started on development of procedures for analysis of the characteristics of generation-recombination-trapping centers in silicon. Supplementary data concerning staff, standards committee activities, technical services, and publications are included as appendixes.

**TN744. Disclosures on: New syntheses of perfluorostyrene and other highly fluorinated derivatives; temperature-, radiation-, and vacuum-resistant magnetic tape; conductometric titration cell; mill work positioner; process for fabricating superconducting microbridges; apparatus for displaying average wind vane or other shaft position; and document numbering machine responsive to a staple in a print area for printing in an alternate area.** D. Robbins and A. J. Englert, Editors, Nat. Bur. Stand. (U.S.), Tech. Note 744, 31 pages (Nov. 1972).

**Key words:** Conductometry; decoding matrix; fluoroolefins; integrator; magnetic sensing probe; magnetic tape; microbridge; numbering machine; perfluorostyrene; shaft position encoder; staple detector; superconducting; synthesis, chemical; titration; wind vane; work positioner.

This Note describes and illustrates seven developments that are believed to embody interesting and unusual solutions to current problems in their fields.

**TN746. Estimates of the nature and extent of lead paint poisoning in the United States.** J. F. Gilsinn, Nat. Bur. Stand. (U.S.), Tech. Note 746, 163 pages (Dec. 1972).

**Key words:** Childhood diseases; estimation; health problems; lead; lead paint; lead paint poisoning; lead poisoning; mathematical modeling; models; urban health problems.

This report evaluates the nationwide magnitude and extent of pediatric lead poisoning resulting from the ingestion of lead-based paint. Estimates are given of the number of children who have elevated blood lead levels (40  $\mu\text{g}$  or more of lead per 100 ml of whole blood) in each of 241 Standard Metropolitan Statistical Areas throughout the country. The mathematical models used to obtain these estimates are documented together with the assumptions and data upon which those models are based. Partial validation of both models and assumptions is also reported.

**TN747. Critical evaluation of data in the physical sciences—A status report on the National Standard Reference Data System, June 1972.** S. A. Rossmassler, Editor, Nat. Bur. Stand. (U.S.), Tech. Note 747, 79 pages (Nov. 1972).

**Key words:** Atomic and molecular data; chemical kinetics; colloid and surface properties; data systems design; information services; mechanical properties; nuclear data; standard reference data; solid state data; thermodynamic and transport properties.

This is a report on the status of the National Standard Reference Data System as of June 1972. Recent activities of the

Office of Standard Reference Data are summarized and future plans are indicated. A complete list of data evaluation projects supported by the Office of Standard Reference Data during Fiscal Year 1972 is included; this list also includes projects which received financial support during an earlier fiscal year, and which are still actively involved in some aspect of data compilation and evaluation, or which are still preparing a product for publication. Progress in data processing and in information services is reviewed. The appendix includes a listing of continuing data centers in the United States and a list of publications resulting from the standard reference data program.

**TN749. The flammable fabrics program 1971.** U.S. Department of Commerce report of activities under the Flammable Fabrics Act 1971, Nat. Bur. Stand. (U.S.), Tech. Note 749, 92 pages (Dec. 1972).

**Key words:** Annual report to Congress; blankets; children's sleepwear; flammability; flammability reduction; mattresses; research; sampling plans; standards; test development; upholstered furniture.

This Annual Report to the Congress, required by the Flammable Fabrics Act, covers calendar year 1971. Specific flammability standards outputs were standards for children's sleepwear in sizes 0 through 6X, a proposed standard for mattresses, and a finding of possible need for amendment of the children's sleepwear standard to add sampling plans for the periodic testing by manufacturers of subject garments and materials. Research included studies, in-house and under contract, on subjects such as the contribution of floor covering systems to fire spread along building corridors and the parameters related to the burning of cotton/polyester blends and of multilayer fabrics. Studies of the feasibility of reducing flammability included the effects of treatments on combustion products and the effects of heavy metal ions on flammability. Test development, in addition to that basic to the standards developments already mentioned, included work on a blanket test, an upholstered furniture test, and on a general apparel test. A series of formal training sessions was initiated to supplement the continuing informal training, presentations, etc. Extensive cooperation was carried out with HEW, the public, industry, and voluntary standards groups.

**TN750. Matches and lighters in flammable fabric incidents: The magnitude of the problem.** J. A. Slater, B. Buchbinder, and H. Tovey, Nat. Bur. Stand. (U.S.), Tech. Note 750, 27 pages (Dec. 1972).

**Key words:** Fabric fires; FFACTS; fire injuries; flammable fabrics; ignition sources; lighters; matches.

Matches and lighters were a major factor in the 1,838 flammable fabric incidents studied for which ignition sources are known. They accounted for 430, almost one-fourth, of the ignitions and led to 375 injuries, of which 57 were fatal. Children and the elderly were the groups most frequently involved in fires started by matches or lighters. Nearly half the incidents involved children under age 11, and two-thirds of these were children under age 6. Forty-four of the 57 fatalities were children under age 11 or adults over 65. The highest fatality rate, 57 percent, was experienced by persons over age 65. The home was the predominant location of fires involving matches and lighters. Of the fabric items ignited by matches and lighters, garments were first to ignite four times as frequently as nonapparel items such as furnishings and bedding. Over one-third of the incidents involved intermediary materials in the ignition sequence. Match ignitions outnumbered lighter ignitions by 6 to 1. Among the 430 match and lighter incidents, fires involving children were overwhelmingly the result of playing with matches and lighters, whereas for persons over age 16, smoking was the single most prevalent activity at the time of ignition.

### 3.13. CONSUMER INFORMATION SERIES

Practical information, based on NBS research and experience, covering areas of interest to the consumer. Easily understandable language and illustrations provide useful background knowledge for shopping in today's technological marketplace.

CIS5. Care of books, documents, prints and films, W. K. Wilson and J. L. Gear, Nat. Bur. Stand. (U.S.), Consum. Inf. Ser. 5, 19 pages (Dec. 1971).

Key words: Films; negatives; paper; photographs; preserva-

tion of records; prints; records; repair of records; storage of records; slides.

This paper describes what the average person can do to care for the books, documents, films and prints that he hopes to preserve for a long time. It tells (1) what *can* be done with respect to storage and simple repair, (2) what *not* to do, such as storage in hot attics and damp basements, (3) when to seek professional help and (4) where to go to find more detailed information.



## 4. TITLES AND ABSTRACTS OF PAPERS PUBLISHED BY OTHERS, 1972

### 4.1. NBS OFFICE OF STANDARD REFERENCE DATA BIBLIOGRAPHY SERIES

The following Bibliography Series are available by purchase from the National Technical Information Service (NTIS), Springfield, Va. 22151 at the prices indicated.

**COM-71-01103. Weekly list of papers on radiation chemistry, index and cumulation**, Vol. IV, Nos. 1-26, Jan. through June 1971, Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame, Aug. 1971, \$6.00.

Key words: Biological systems; ESR; hot atom chemistry; luminescence; photochemistry; polymers; radiation chemistry; radiation chemistry theory.

The Radiation Chemistry Data Center, as part of its operations, collects, keywords, and stores literature of fundamental radiation chemistry and several related fields. Since 1968 references to this literature have been stored in computer files. These files have been used for retrospective researches and for the Weekly List of Papers on Radiation Chemistry which has been used as a current-awareness aid by radiation chemists since 1968. This index to and cumulation of entries in the Weekly List of Papers on Radiation Chemistry for the period of January through June 1971 is intended as a guide to the recent literature and as a searching tool for those who would find a printed index valuable.

**COM-72-10014. Kondratiev, V. N., Rate constants of gas phase reactions**, Translated by L. J. Holtschlag and Edited by R. M. Fristrom, 433 pages, Jan. 1972 (Johns Hopkins University, Applied Physics Laboratory, Silver Spring, Md.), \$8.50.

Key words: Atom reactions; compilation; critical evaluation; gas phase reactions; radical reactions; rate constants.

This survey of the kinetics of bimolecular and termolecular reactions covers the literature to the end of 1969. Gas-phase reactions of neutral particles have been surveyed, rate constants are presented in consistent units and a number of reactions have been critically evaluated. A table of equilibrium constants has been added to the English edition as well as a bibliography of rate constant compilations and sources of evaluated kinetic information.

**COM-72-10266. Index and cumulative list of papers on radiation chemistry**, Vol. IV, Nos. 27-52, July through Dec. 1971,

Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame, Jan. 1972, \$6.00.

Key words: Biological systems; ESR; hot atom chemistry; luminescence; photochemistry; polymers; radiation chemistry; radiation chemistry theory.

The Radiation Chemistry Data Center, as part of its operations, collects, keywords, and stores literature of fundamental radiation chemistry and several related fields. Since 1968 references to this literature have been stored in computer files. These files have been used for retrospective researches and for the Weekly List of Papers on Radiation Chemistry which has been used as a current-awareness aid by radiation chemists since 1968. This index to and cumulation of entries in the Weekly List of Papers on Radiation Chemistry for the period of July through December 1971 is intended as a guide to the recent literature and as a searching tool for those who would find a printed index valuable.

**COM-72-10621. Index and cumulative list of papers on radiation chemistry**, Vol. V, Nos. 1-26, Jan. through June 1972, Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame, Jan. 1972, \$6.00.

Key words: Biological systems; ESR; hot atom chemistry; luminescence; photochemistry; polymers; radiation chemistry; radiation chemistry theory.

The Radiation Chemistry Data Center, as part of its operations, collects, keywords, and stores literature of fundamental radiation chemistry and several related fields. Since 1968 references to this literature have been stored in computer files. These files have been used for retrospective researches and for the Weekly List of Papers on Radiation Chemistry which has been used as a current-awareness aid by radiation chemists since 1968. This index to and cumulation of entries in the Weekly List of Papers on Radiation Chemistry for the period of January through June 1972 is intended as a guide to the recent literature and as a searching tool for those who would find a printed index valuable.

## 4.2. OTHER NBS PAPERS PUBLISHED IN NON-NBS MEDIA

Reprints from the journals listed in this section may often be obtained directly from the authors. See page 2, section 1.5 for additional information.

**12381.** Ambler, E., **Measurement standards, physical constants, and science teaching**, *Sci. Teacher* 38, No. 8, 63-71 (Nov. 1971).

Key words: Measurement standards; physical constants; science teaching.

Man's intuitive ability to perceive and recognize such concepts as temperature and distance is well-developed even before his formal education begins. The inherited internal measurement, or sensory, systems are extremely sensitive and lead to a direct awareness and comprehension of the physical world in ways we do not yet completely understand. Man's need to measure and quantify more formally and less intuitively goes back as far as recorded history itself.

Man's ability to measure physical quantities in a coherent and rational manner grew with the development of physics as a science. Indeed our very basic concepts of the nature of the physical world, such as mass, time, temperature, entropy and so on, related as they are through the laws of physics, provide the basis for a coherent and internationally recognized system of measurement. The need to root our measurement system deeply in our understanding of natural phenomena was recognized from the very outset of organized metrology ("un Nouveau système métrique") long before our understanding of relativity, atomic structure, quantum theory and the significance of fundamental physical constants, such as the speed of light, Planck's quantum of action and the basic unit of electric charge, developed. Yet the same general principle applies today as it did two hundred years ago, as we strive to incorporate the latest developments, such as the coherent light from lasers and the coherent electric currents of superconduction, into a better physical measurement system.

As matters now stand our ability to measure physical quantities is extremely refined and has been extended far beyond the ranges of intuitive perception, so that we can measure the diameter of atoms that we cannot see, and the distance to the moon that we cannot reach. It is strange that some quantities that were relatively recently only poorly understood, such as electric current, are now almost universally understood and are measured with utmost confidence and precision every day, while in other quantities, such as the difference between sound that is pleasing and sound that is annoying, to which man has surely responded since time immemorial, we measure with much less unanimous confidence. Yet now we are called upon to measure more complex quantities such as noisiness of sounds in connection with measuring and controlling our environment. We are faced with linking physical phenomena, which we understand quite well, with human response which we understand less well. It seems fairly clear that a deeper scientific study of the workings of man's senses and an understanding of reasonable limits of his adaptability to variations in the stimulation of his senses is a challenging field in which there is great need to devise new methods of meaningful measurement.

**12382.** Blandford, J. M., Baker, H. A., **Sewing threads for the apparel industry**, *Apparel Research Foundation, Inc., Washington, D.C.*, pp. 1-153 (May 15, 1971).

Key words: Apparel industry; industry, apparel; performance, sewing thread; properties, sewing thread; quality

control, sewing threads; sewing threads; testing programs, sewing thread tests, sewing thread; thread properties; threads, sewing.

The objectives, development, and achievements of the National Bureau of Standards (NBS) Sewing Thread Project, carried out in collaboration with The Apparel Research Foundation, Inc. (ARF) are discussed.

The results of two questionnaire-surveys conducted among thread and apparel companies are summarized, as are the opinions expressed by thread and apparel manufacturers on industry-wide adoption of a uniform thread-sizing system.

Included are tabulations, graphs, and a statistical analysis of NBS tests of threads representative of those currently used by the apparel industry: soft and mercerized cotton; core and spun polyester; and nylon.

Testing programs for evaluating (1) the quality of threads purchased by the apparel manufacturer; and (2) the performance of threads in the apparel product, are discussed in detail. The following information is tabulated: testing equipment; properties which may be determined by its use; testing procedures and evaluation materials employed; and sources of supply and approximate prices of the equipment and evaluation materials. Supplementing the text are reprints of the 21 referenced test methods.

**12383.** Brandenberger, H., Hadron, F., Halford, D., Shoaf, J. H., **High quality quartz crystal oscillators: Frequency domain and time domain stability**, *Proc. 25th Frequency Control Annual Symp., Atlantic City, N.J., Apr. 26-28, 1971*, pp. 226-234 (Electronic Industries Association, Washington, D.C., Apr. 1971).

Key words: Allan variance; flicker of phase noise; frequency stability; oscillator noise models; phase noise spectral density; quartz crystal oscillator; time domain stability.

We measured the frequency stability of a pair of commercial 5-MHz quartz crystal oscillators which incorporate improved electronic design for enhanced short-term stability. The spectral density (frequency domain) of the phase noise, per oscillator, measured by each of our two laboratories, is

$$S_{\phi\phi} = + (10^{-11.8} \text{ radians}^2 \text{ Hz}^2)(1/f^3) + (10^{-12.5} \text{ radians}^2)(1/f) + (10^{-14.4} \text{ radians}^2 \text{ Hz}^{-1})f^0.$$

over the range of about  $10^{-2}$  Hz to  $10^{+3}$  Hz.

**12384.** Brown, D. W., Lowry, R. E., Wall, L. O., **Radiation-induced polymerization at high pressure of 2,3,3,3-tetrafluoropropene in bulk and with tetrafluoroethylene**, *J. Polymer Sci. 9, Part A-1*, 1999-2007 (1971).

Key words: Polymerization; pressure; radiation-induced; tetrafluoroethylene; 2,3,3,3-tetrafluoropropene.

The radiation-induced polymerization of 2,3,3,3-tetrafluoropropene was studied as a function of temperature ( $22 - 100^\circ\text{C}$ ) and pressure (autogenous to  $10^4$  atm). Rates have varied 100-fold for the same reaction conditions probably because of trace impurities. The most rapidly polymerizing material has a rate of 4.5%/hr at 6000 atm,  $22^\circ\text{C}$ , and 1500 rad/hr. The activation enthalpy and volume are 4 kcal/mole and  $-13$  cc/mole, respectively. Rates are proportional to the square root of the radiation intensity. Degrees of polymerization varied



between  $2 \times 10^3$  and  $2 \times 10^6$ . In copolymerization with tetrafluoroethylene the reactivity ratios at 22 °C and 5000 atm are 0.37 (the ratio for addition to the tetrafluoroethylene-ended radical) and 5.4 (the ratio for addition to the copolymerization of other fluorine-containing monomers with tetrafluoroethylene shows that they generally disfavor incorporation of the latter).

**12385.** Clifton, J. R., **The infrared spectra of supposed  $\alpha$  and  $\beta$  forms of calcium sulphate hemihydrate**, *Nature (London), Phys. Sci.* **232**, No. 32, 125-126 (Aug. 9, 1971).

Key words:  $\alpha$ -CaSO<sub>4</sub>·1/2H<sub>2</sub>O;  $\beta$ -CaSO<sub>4</sub>·1/2H<sub>2</sub>O; gypsum; infrared spectra; lattice water.

The infrared absorption spectra of supposed  $\alpha$  and  $\beta$  forms of calcium sulfate hemihydrate were measured from 580 to 4000 cm<sup>-1</sup>, using doped potassium bromide pellets and mineral oil mulls.

It was impossible to differentiate between the two supposed forms of calcium sulfate hemihydrate because their infrared spectra were closely similar. The spectra of the supposed forms dispersed in potassium bromide consisted of 13 absorptions and the maximum difference in position between analogous bands of the two spectra was 5 cm<sup>-1</sup> while 8 absorptions had identical frequencies. Both supposed forms gave the same spectral features when made into mineral mulls.

Because of the high frequencies of  $\nu_1$ (H<sub>2</sub>O), 3528 cm<sup>-1</sup>, and  $\nu_3$ (H<sub>2</sub>O), 3604 cm<sup>-1</sup>, for calcium sulfate hemihydrate, it has been proposed that the water molecules are only interstitially held in the hemihydrate.

**12386.** Coriell, S. R., Hardy, S. C., Sekerka, R. F., **A non-linear analysis of experiments on the morphological stability of ice cylinders freezing from aqueous solutions**, *J. Crystal Growth* **11**, 53-67 (May 1971).

Key words: Cylinder; ice; morphology; non-linear; stability; surface tension.

A non-linear theory of morphological stability of a solid circular cylinder growing in a supercooled melt is developed and applied to recent experiments on the growth of ice cylinders in distilled water and in aqueous solution. The cylinders develop  $\Phi$  perturbations in the circular shape and  $z$  perturbations parallel to the axes of the cylinders. The theory successfully predicts the growth rate of the  $z$  perturbations. The non-linearity arises because the  $\Phi$  perturbations have grown to a substantial size before the  $z$  perturbations are measured. From an analysis of the  $z$  perturbation growth rates, a value of 25 mJ/m<sup>2</sup> is obtained for the ice-water surface tension on surfaces parallel to the  $c$ -axis; the corresponding value obtained from a less-satisfactory linear analysis was 22 mJ/m<sup>2</sup>.

**12387.** Coxon, B., Schaffer, R., **Characterization and quantitative analysis of D-glucose for use in clinical analysis**, *Anal. Chem.* **43**, No. 12, 1565-1570 (Oct. 1971).

Key words:  $\alpha$ -D-glucose; anomerization;  $\beta$ -D-glucose; calorimetry; clinical analysis; differential scanning calorimetry; equilibration; gas chromatography; polarimetry; proton magnetic resonance spectroscopy.

The results from analysis of  $\alpha$ -D-glucose and  $\beta$ -D-glucose by a variety of spectrometric, chromatographic, and polarimetric techniques are presented and discussed. The apparent values of purity obtained for  $\alpha$ -D-glucose by differential scanning calorimetry are discussed in relation to the content of  $\beta$  anomer as determined by gas chromatography and proton magnetic resonance spectroscopy. It is shown that, during melting, both  $\alpha$ -D-glucose and  $\beta$ -D-glucose anomerize rapidly to give an equilibrated mixture of these anomers.

**12388.** Danos, M., **One physicist's view of special functions**, (Proc. SIAM National Meeting, Washington, D.C., June 10-12, 1969), Chapter in *Studies in Applied Mathematics* **6**, pp. 18-29 (1970).

Key words: Analytical continuation; electron scattering; potential scattering; recoupling coefficients; Regge poles; special functions.

The need for presently unavailable information is illustrated with three examples taken from physics problems of present interest. They involve both the evaluation of integrals over special functions and the analytic continuation in one or several variables of diverse quantities which can be defined by differential or difference equations. Of particular interest would be the solution of the Schrödinger equation for the scattering of a particle in a Yukawa potential.

**12389.** deWit, R., **Relation between dislocations and disclinations**, *J. Appl. Phys.* **42**, No. 9, 3304-3308 (Aug. 1971).

Key words: Burgers vector; crystal; disclination; dislocation; distant parallelism; hexagonal; wedge.

The theory of disclinations contains the equation  $\partial_i \alpha_{ij} + e_{jmn} \theta_{mn} = 0$ , where  $\alpha$  and  $\theta$  are the dislocation and disclination density tensors, respectively. This expression is interpreted to mean that dislocations can end on twist disclinations. A concrete example in a hexagonal crystal is discussed to illustrate this concept. It contains a 60° wedge disclination normal to the basal plane. By basic geometrical construction it is shown how a dislocation can be made to end on a jog in the wedge disclination. This jog is a small segment of twist disclination. Several ramifications of this concept are that disclinations can act as sources and sinks of dislocations, that dislocations change their Burgers vectors as they glide around disclinations, that a dislocation which crosses a disclination remains connected to it by a dislocation, that dislocations encircling a disclination must have a node, and that the local Burgers vector is not conserved on following a dislocation around a disclination.

**12390.** Dibeler, V. H., **Photoionization studies and thermodynamic properties of some halogen molecules**, (Proc. Intern. Conf. on Mass Spectroscopy, Kyoto, Japan, Sept. 6-13, 1969), Chapter in *Recent Development in Mass Spectroscopy*, K. Ogata and T. Hayakawa, eds., pp. 781-790 (University of Tokyo Press, Tokyo, Japan, 1970).

Key words: Chlorine monofluoride; dissociative ionization; fluorine; heats of formation; hot bands; hydrogen fluoride; ion pairs; mass spectrometry; molecular ionization; photoionization; vacuum ultraviolet.

Mass spectra and ion yield curves for molecular and dissociative ionization processes are measured for fluorine, hydrogen fluoride, chlorine, and chlorine monofluoride by means of a combined vacuum uv monochromator and mass spectrometer. Ionization and dissociation energies and heats of formation of the molecules are obtained and compared with values derived from thermochemical and spectroscopic studies.

**12391.** Dibeler, V. H., Walker, J. A., McCulloh, K. E., **Dissociation energy of fluorine**, *J. Chem. Phys. Letters to Editor* **50**, No. 10, 4592-4593 (May 15, 1969).

Key words: Dissociation energy; fluorine; mass spectrometry; photoionization; vacuum ultraviolet.

Photoionization and mass analysis are used to determine the dissociation energy and estimated uncertainty,  $D^0(F_2) = 1.34 \pm 0.03$  eV. The molecular ionization energy is also determined to be  $15.69 \pm 0.01$  eV. Both  $F^+$  and  $F^-$  ions are obtained by the ion-pair process.

**12392.** Dibeler, V. H., Walker, J. A., McCulloh, K. E., **Photoionization study of the dissociation energy of fluorine and the heat of formation of hydrogen fluoride**, *J. Chem. Phys.* **51**, No. 10, 4230-4235 (Nov. 15, 1969).

**Key words:** Bond dissociation energies; fluorine; heats of formation; hydrogen fluoride; ionization thresholds; mass spectra; photoionization; vacuum uv.

Mass spectra and photoionization yield curves are obtained for the molecular and atomic ions of fluorine and hydrogen fluoride. The atomic ions of both molecules are formed by ion-pair and by dissociative ionization processes. The  $F_2^+$  curve has a weak onset at 15.58 eV, ascribed to a hot band, followed by an abrupt, intense onset at 15.69 eV, ascribed to the  $0-0$  transition. Several broad bands of autoionization are observed. The onset of the dissociative ionization process occurs at 18.76 eV, from which we calculate  $D_0^\circ(F_2)=1.34\pm 0.03$  eV (30.9 kcal mol<sup>-1</sup>). The only observed ion-pair process is spin forbidden, producing  $F^+(\text{^3P})+F^-(\text{^1S})$ , for which the thermodynamic threshold is not reached. The  $HF^+$  curve has a slightly tailing onset at 15.92 eV. No  $F^+$  ion is observed. The dissociative ionization process yielding  $H^+$  occurs at 19.34 eV, permitting the calculation of  $D_0^\circ(HF)=5.74$  eV, and  $\Delta H_f^\circ(HF)=-2.83\pm 0.03$  eV ( $-65.3$  kcal mol<sup>-1</sup>). Identical ion-pair curves have a threshold at 15.87 eV resulting in  $EA(F)=3.47$  eV. The indicated uncertainties are estimated limits of error.

**12393.** Dibeler, V. H., Walker, J. A., McCulloh, K. E., **Threshold for molecular photoionization of bromine**, *J. Chem. Phys.* **53**, No. 12, 4715-4716 (Dec. 15, 1970).

**Key words:** Bromine; hot-bands; mass spectrometry; molecular ionization; photoionization.

This brief communication reports on a photoionization measurement of the threshold for molecular ionization of bromine. Ionization of vibrationally-excited molecules is resolved from the  $0,0$  transition and a value of  $I(Br_2)=10.52\pm 0.01$  eV is obtained.

**12394.** Douglas, C. A., **A survey of the use of flashing lights in aviation**, *Proc. Intern. Symp. on Perception and Application of Flashing Lights*, London, England, Apr. 1971, pp. 251-270 (Adam Hilger Ltd., London, England, Apr. 1971).

**Key words:** Aerodrome lighting; aircraft lighting; anti-collision lights; beacons; effective intensity; flashing lights.

Flashing lights have been used as beacons since the first days of night flying. They are also used as identification lights in approach and runway light systems. They have been used for many years to mark obstructions and other hazards by night and are now being introduced as daytime markers. Flashing lights have been used since the 1940's to supplement the navigation lights on aircraft. Photometric performance of these lights is usually specified in terms of steady state intensity and minimum flash duration or in terms of the candela seconds in the flash. Use of the integral form of the Blondel-Rey relation was introduced in the 1950's and use of this relation is increasing.

**12395.** Douglas, T. B., **Summary of recent thermodynamic measurements by calorimetric, transpiration, mass spectrometric microwave, and infrared techniques**, *Proc. Conf. Interagency Chemical Rocket Propulsion Group, Thermochemistry Working Group, Huntington Beach, Calif., Mar. 25-27, 1968, 6th Meeting Bulletin 173*, **1**, 93-104, (Chemical Propulsion Information Agency, The Johns Hopkins University, Applied Physics Laboratory, Silver Spring, Md., Aug. 1968).

**Key words:** Absorption spectrometry; calorimetry; mass spectrometry; propulsion applications; thermodynamic measurements; transpiration equilibria.

This paper summarizes recent precise thermodynamic measurements, completed or in progress, by several research groups at the National Bureau of Standards (NBS). The heats of formation of  $ClF_3(g)$  and  $BeO(c)$  are being measured by reaction calorimetry. "Heat-capacity calorimetry" has been completed at low temperatures on  $Be_3N_2(c)$  and on  $BeO(c)$  (larger crystals than usual), and at high temperatures on tungsten (to 2600 K) and on  $BeO\cdot Al_2O_3(c,l)$  (to 2350 K). A new technique of fast dynamic calorimetry at high temperature has become operational for millisecond heating, with preliminary measurements on molybdenum and other electrically conducting refractories. Transpiration data on the  $AlF_3-AlCl_3$  system have been analyzed to give the heats of formation of  $AlF_2Cl(g)$  and  $AlFCl_2(g)$ . High-temperature mass spectrometry is underway on the  $BeF_2-BeCl_2$  and the  $BeO-H_2O$  systems. In the high-temperature microwave and the matrix-isolation infrared investigations of the alkali-hydroxide molecules, spectra have recently been observed and analyzed for  $RbOH$  (microwave and infrared) and for  $NaOH$  (infrared).

**12396.** Driscoll, R. L., Olsen, P. T., **Compensation of earth's field variations by field controlled rubidium oscillator**, *Rev. Sci. Instr.* **42**, No. 10, 1427-1431 (Oct. 1971).

**Key words:** Absorption cell; earth's magnetic field; Helmholtz coil; magnetometer; optical pumping; resonance line; rubidium oscillator; solenoid.

The east-west variations of the earth's magnetic field over the working volume of the NBS precision solenoid are being canceled out by a closed loop system featuring a field controlled rubidium oscillator. The rubidium oscillator and solenoid are sufficiently separated in distance and do not affect each other's operation. Each system is enclosed in three-dimensional Helmholtz coils. Vertical and north-south components of earth's field are canceled. An east-west bias field is provided for rubidium oscillator operation at 10 kHz. The output of a phase sensitive detector locked to the 10 kHz frequency standard provides current for the electrically series connected east-west Helmholtz coils at both locations. The magnitude of this current is proportional to the phase difference of oscillator and reference. The full range of compensation is 100 nT. The rate of compensation is limited by a time constant of 0.002 sec, an adequate rate for most disturbances. To the extent that the two separated components of the closed loop system can be oriented directionally the same at any given time, the earth's field east-west variation is compensated exactly.

**12397.** Ekstrom, M. P., McCaa, W. D., Jr., Nahman, N. S., **The measured time and frequency response of a miniature superconducting coaxial line**, *IEEE Trans. Nucl. Sci.* **NS-18**, No. 5, 18-25 (Oct. 1971).

**Key words:** Cable; step response; superconducting transmission line; time domain deconvolution.

A miniature superconducting 52 ohm coaxial transmission line 278 meters long, having a lead outer conductor (0.129 cm id), a teflon dielectric, and a niobium center conductor (0.038 cm), has been measured in both the time and frequency domains. The observed system step response (10% - 90%) times were 1.5  $\mu s$  at room temperature, 375 ns at 77 K, and 255 ps at 4.2 K. The system step response data for 4.2 K was processed by a numerical system identification routine to determine the step response of the miniature superconducting line; the processed data gave a 220 ps risetime. Although the observed step responses at 4.2 K were smooth transitions, the observed swept frequency (0.1 GHz - 12 GHz) attenuation at 4.2 K was a quasi-periodic function of frequency, which indicated that the nonuniformity of the superconducting line was significant. For example, near 5 GHz and at 4.2 K, the attenuation minimum was 1.1 dB while about



0.5 MHz away the attenuation was 5 dB. By making normal conductivity measurements of the Nb conductor and incorporating the results into the two fluid model, the uniform line attenuation for 5 and 10 GHz was calculated with the classical and anomalous limits. The lowest observed attenuation values in the vicinity of 5 and 10 GHz fell between the computed classical and anomalous limit attenuation values.

**12398.** Forthofer, R. J., **Developing standards technology for automotive braking systems**, *Proc. 1969 18th Annual Meeting Standards Engineers Society, Washington, D.C., Sept. 15-17, 1969*, pp. 27-42 (Sept. 1969).

Key words: Automotive; brake; brake fluid; brake lining; standards; testing.

The Office of Vehicle Systems Research (OVSF) of the National Bureau of Standards, U.S. Department of Commerce, is concerned with the research, development, testing and evaluation necessary to provide the technical basis for recommended safety performance standards issued by the National Highway Safety Bureau of the Department of Transportation.

This paper discusses briefly the history of the Government's interest in automotive braking safety standards. Problems associated with the collection of research data for the performance of brake systems, brake linings, and brake fluid are discussed in more detail. The author comments on the direction that research is expected to take in the 1970's.

**12399.** Freeman, D. H., Enagonio, D. P., **Interactive gel networks for organic separations**, *Nature (London), Phys. Sci.* **230**, 135-136 (Apr. 1971).

Key words: Chromatography; interactive gel networks; liquid chromatography; organic separations.

Conventional organic networks, such as crosslinked polyvinylpyridine, can be used or modified so that chemical interactions of various specific types are obtained. They show excellent resolution and high capacity. The chromatographic properties are related to complexative interactions whose understanding in liquid media is independently established.

**12400.** Geist, J., **Note on the quality of freezing point blackbodies**, *Appl. Opt.* **10**, No. 9, 2188-2190 (Sept. 1971).

Key words: Blackbody; emissivity; freezing point blackbody; heat pipe blackbody; quality.

It is shown that for freezing point blackbodies whose wall materials have thermal radiative properties which are independent of wavelength, a quantity can be defined which satisfies all of the intuitive ideas of the concept of the quality of the blackbody and which satisfies an integral equation which provides physical insight into the interaction of the reflectance and thermal resistance of the wall material of the blackbody in reducing its quality from unity.

**12401.** Hermach, F. L., **Testing hospital electric equipment for safe performance**, *Proc. National Research Council Workshop on Electric Hazards in Hospitals, Washington, D.C., Apr. 4-5, 1968*, pp. 175-177 (National Academy of Sciences, Washington, D.C., 1970).

Key words: Electric equipment; electrical safety; hospital safety; leakage currents; testing; test sets.

Electric equipment for use on patients must be evaluated to determine if it meets the requirements of safety codes—otherwise the codes are of little value. This can best be done by safety-testing labs which follow established test methods to determine compliance with broad performance requirements of such codes. A test set to which the user can connect electric equipment to

determine if leakage currents are less than allowable limits would be valuable additional protection, particularly in the interim period before approved equipment is available.

**12402.** Herron, J. T., **Mass spectrometric studies of atomic and free radical reactions**, *Advan. Mass Spectrometry* **5**, 453-461 (1971).

Key words: Atomic; chemical kinetics; free radicals; mass spectrometry; mechanism; review.

The applications of mass spectrometry to the study of the kinetics and mechanisms of atomic and free radical reactions in the gas phase are reviewed.

**12403.** Hudson, R. P., Mangum, B. W., **Effects of applied magnetic fields on cooperative Jahn-Teller transition temperatures of DyAsO<sub>4</sub> and DyVO<sub>4</sub>**, *Physics Letters* **36A**, No. 3, 157-158 (Aug. 30, 1971).

Key words: Jahn-Teller effect; magnetic susceptibility.

We have measured the effects of applied magnetic fields on the cooperative Jahn-Teller transition temperatures of DyAsO<sub>4</sub> and DyVO<sub>4</sub>. We find that even relatively weak fields produce a very pronounced increase in the transition temperature of DyAsO<sub>4</sub>.

**12404.** Hudson, P. A., Saulsbery, L. F., **An adjustable-slot-length UHF coaxial coupler with decade bandwidth**, *IEEE Trans. Micro. Theory Tech.* **MTT-19**, No. 9, 781-783 (Sept. 1971).

Key words: Attenuator; directional coupler, coaxial; power measurement, rf.

A coaxial directional coupler has been developed which allows adjustment of the length of the coupling slot to  $\lambda/4$  or  $3\lambda/4$  throughout the frequency range 0.3 to 8.5 GHz. Coupling is flat to within 0.05 dB from 0.3 to 3 GHz ( $\lambda/4$  mode) and 0.1 dB from 0.9 to 8.5 GHz ( $3\lambda/4$  mode). The coupler has 50-dB coupling, 30- to 40-dB directivity and was designed primarily for high power measurement (1 to 1000 W) using a low-power meter on the sidearm. The VSWR for the two modes of operation is 1.02 to 1.05. Five octave bandwidth-type couplers would be required to cover this same frequency range.

**12405.** King, D. A., Madey, T. E., Yates, J. T., Jr., **Interaction of oxygen with polycrystalline tungsten. II. Corrosive oxidation**, *J. Chem. Phys.* **55**, No. 7, 3247-3253 (Oct. 1, 1971).

Key words: Adsorption; chemisorption; corrosion; flash desorption; oxidation; oxygen; tungsten; tungsten oxides.

The kinetics of formation of a corrosive oxide layer of apparently unlimited thickness during the interaction of oxygen with a polycrystalline tungsten filament at temperatures between 500 and 1000 K has been investigated by line-of-sight flash desorption mass spectrometry. The major desorption product from this multilayer oxide film is WO<sub>2</sub>, which desorbs over the temperature range 1000 to 1300 K. The rate of formation of the oxide film was shown to be directly proportional to the oxygen gas phase pressure at pressures  $\leq 10^{-4}$  torr. A study of the temperature dependence of the oxidation rate revealed that the formation of the WO<sub>2</sub>-producing oxide layer proceeds through two distinct steps: these occur subsequent to the first three stages in the interaction of oxygen with W characterized in Paper I. In the final stage of oxidation, the rate is shown to be independent of the thickness of the oxide film. The results are in qualitative accord with the theoretical model of Mott. Desorption of the oxide film is a zero order process, with a desorption activation energy of 420 kJ mol<sup>-1</sup>.

**12406.** Koonce, C. S., Mangum, B. W., Thornton, D. D., **Low temperature properties of DyPO<sub>4</sub> in a magnetic field**, *Proc. 12th Intern. Conf. on Low Temperature Physics, Kyoto, Japan*,

Sept. 4-10, 1970, pp. 705-707 (Keigaku Publishing Co., Japan, Mar. 1971).

Key words: Antiferromagnetic; dipolar interaction;  $\text{DyPO}_4$ ; low temperature; magnetic field; paramagnetic.

The magnetization and the peaks in the heat capacity at constant applied field of  $\text{DyPO}_4$ , a material for which the Ising model is particularly appropriate, have been measured, and compared with a Bethe-Peierls approximation including dipolar interactions.

**12407.** Kranbuehl, D. E., **Atomic, molecular, and ionic interactions**, *Dig. Lit. Dielectrics* **33**, No. 2, 84-118 (1969).

Key words: Dielectric; ionic; polarizability; relaxation.

A review of those papers in the 1969 literature on dielectrics which make a significant contribution toward understanding the fundamental dielectric properties of atoms, molecules and ions.

**12408.** Kranbuehl, D. E., Verdier, P. H., **Stochastic molecular model studies of the relaxation of vector end-to-end length in polymer chains**, *Am. Chem. Soc. Polymer Preprints* **12**, No. 2, 625-628 (1971).

Key words: End-to-end length; excluded volume; Monte Carlo; polymer chain dynamics; relaxation.

The effects of excluded volume interactions upon the dynamical behavior of random-coil polymer chains are studied by obtaining autocorrelation functions for the vector end-to-end length of lattice model chains of 9, 15, 33, and 63 beads by a Monte Carlo simulation technique. The configuration of the polymer chain,  $N-1$  units long, is represented by a string of  $N$  connected points on a 3-dimensional cubic lattice. Excluded volume is accounted for by not allowing two beads to occupy the same lattice site. It is found that the relaxation of vector end-to-end length for a lattice chain with excluded volume varies substantially from that of a lattice chain without excluded volume. Relaxation of the vector end-to-end length requires from four to seven times as long as relaxation of its square, contrary to the predictions of simple models without excluded volume effects. This behavior suggests that the ratio of the relaxation time of vector end-to-end length to that of its square is a measure of the presence or absence of excluded volume effects.

**12409.** Kuriyama, M., Alexandropoulos, N. G., **On the relationship between x-ray inelastic scattering and absorption spectra**, *J. Phys. Soc. Japan* **31**, No. 2, 561-562 (Aug. 1971).

Key words: Compton scattering; plasmon scattering; Raman scattering; relation between spectra; x-ray absorption; x-ray inelastic scattering.

The cross section for x-ray inelastic scattering from crystals has been derived from first principles to explain the coexisting Compton and Raman scattering in solids. This derivation makes it possible to express the inelastic scattering cross section in terms of the current correlation of electrons in a crystal. The criterion for having a distinct Raman scattering is obtained through the dependence of the current correlation on the momentum transfer.

**12410.** Lee, J. N., Moos, H. W., Mangum, B. W., **Magnetic properties of  $\text{TbPO}_4$ , a canted antiferromagnet**, *Solid State Commun.* **9**, No. 13, 1139-1141 (1971).

Key words: Antiferromagnet; canted antiferromagnet; heat capacity; magnetic moment; magnetic susceptibility; metamagnet; optical spectroscopy;  $\text{TbPO}_4$ .

The magnetic properties of  $\text{TbPO}_4$  at low temperatures have been investigated by high resolution optical spectroscopy, magnetic susceptibility, magnetization, and heat capacity measurements.  $\text{TbPO}_4$  orders antiferromagnetically into a canted spin structure with zero net moment at 2.17 K. Metamagnetic behavior is observed. A magnetically induced lattice distortion mechanism is probably responsible for the detailed behavior.

**12411.** Manning, J. R., **Correlation factors for diffusion in non-dilute alloys**, *Phys. Rev. B* **4**, No. 4, 1111-1121 (Aug. 15, 1971).

Key words: Alloys; atom jump frequencies; binary alloys; correlation factor; diffusion; multicomponent alloys; random alloy model; vacancies.

Correlation factors for diffusion in binary and multicomponent alloys are calculated for a random-alloy model with diffusion by a vacancy mechanism. This model, which should apply best for nondilute alloys, assumes that atoms and vacancies are randomly distributed and that suitable average values can be used to represent the actual atom and vacancy jump frequencies in the crystal. In alloys, both atoms and vacancies follow correlated walks. Also, the atom correlation factors are influenced by the nonrandom motion of the vacancies. Thus, in order to treat correlation effects in concentrated alloys properly, one must consider not only the correlation factors  $f_i$  for diffusion of atoms but also the correlation factor  $f_v$  for diffusion of vacancies. In specific calculations, one also must find the partial correlation factors  $f_i^j$  for diffusion of vacancies by exchange with atoms of the particular species  $i$ . Analytic expressions for all of these correlation factors are calculated. These equations can be expressed directly in terms of the measurable tracer-diffusion-coefficient ratios  $D_i^*/D_v^*$  with no unknown jump frequencies appearing. The calculations also yield a forbidden region in the plot of diffusion-coefficient ratio as a function of alloy composition, with correlation factors going to zero at the boundary of this region. Specific applications to binary alloys are discussed.

**12412.** Marzetta, L. A., **A high-performance phase-sensitive detector**, *IEEE Trans. Instr. Meas* **IM-20**, No. 4, 296-301 (Nov. 1971).

Key words: Op amp; operational amplifier; operational rectifier; phase-sensitive detector; signal extraction ratio.

A phase-sensitive detector is described that enables the retrieval of signals submerged 90 dB (voltage) below the noise level. Operation over four decades of signal amplitude (a full-scale linearity error of 0.01 percent) is possible for a frequency range of 0–150 Hz. Design features are offered allowing an experimenter to construct the device from inexpensive components and be assured a predictable performance.

**12413.** Mason, H. L., **Pounds, atoms, papers, and laws**, *Instrument Society of America Silver Jubilee International Conference and Exhibit, Oct. 26-29, 1970, Philadelphia, Pa.*, **25**, Part II, Paper 70-662, 1-5 (1970).

Key words: Calibration; instrument specifications; international standards; measurement history; measuring instruments; physical constants; physical standards.

Reviews three centuries, from William Penn to Richard Simpson, in the development of four kinds of technical standards—physical artifacts, natural phenomena, written agreements, and legal codes. Traces the influence of industrial practices, governmental agencies, and international organizations, on standards which specify quantities, and commercial products.

**12414.** Mighell, A. D., Santoro, A., Donnay, J. D. H., **Reduced cells**, Chapter in *International Tables for X-Ray Crystallog-*



raphy, N. F. Henry and K. Lonsdale, eds., II, 530-535 (The Kynoch Press, Birmingham, England, 1969).

**Key words:** Bravais lattice; identification; reduced cells; transformation matrix.

Tables and text are given that make it possible to determine the reduced cell for any lattice. Finally, a detailed table is presented which establishes the relationship of each of the 44 reduced cell types to one of the Bravais lattices.

**12415.** Milligan, D. E., Jacox, M. E., **Matrix-isolation study of the interaction of electrons and alkali metal atoms with various nitrogen oxides. Infrared spectra of the species  $\text{NO}^-$ ,  $\text{NO}_2^-$ , and  $\text{N}_2\text{O}_2^-$** , *J. Chem. Phys.* **55**, No. 7, 3404-3418 (Oct. 1, 1971).

**Key words:** Alkali metal reactions; charge transfer; electron attachment; infrared spectrum; matrix isolation;  $\text{NO}^-$ ;  $\text{NO}_2^-$ ;  $\text{N}_2\text{O}_2^-$ ;  $\text{O}^-$  reactions.

The infrared spectra which result when samples of  $\text{NO}_2$  are codeposited with the various alkali metals in an argon matrix at 4 or at 14 K are consistent with the occurrence of strong charge-transfer interaction. In addition to isolated  $\text{NO}_2^-$ , previously identified in this system, ion pairs of general formula  $\text{M}_x^+\text{NO}_2^-$  are stabilized. When NO is substituted for  $\text{NO}_2$ , the infrared spectrum of the initial deposit shows an absorption between 1350 and 1375  $\text{cm}^{-1}$  which can be assigned to the  $\text{NO}^-$  stretching fundamental of  $\text{M}_x^+\text{NO}^-$  ion pairs, in good agreement with the vibrational spacing recently reported for ground-state  $\text{NO}^-$  in the gas phase. Weak charge-transfer interaction occurs between alkali-metal atoms and  $\text{N}_2\text{O}$  in an argon matrix environment. Results of the present experiments can be explained by postulating that the upper, predominantly ionic state of the charge-transfer complex decomposes producing  $\text{O}^-$ , which may diffuse through the matrix. A new absorption which appears at 1205  $\text{cm}^{-1}$  has tentatively been assigned to  $\nu_4(b_1)$  of a planar  $\text{O}_2\text{N}=\text{N}^-$  anion. In studies of the interaction of sodium atoms with Ar: $\text{NO}:\text{N}_2\text{O}$  mixtures, mercury-arc irradiation of the sample leads to the appearance not only of the  $\text{N}_2\text{O}_2^-$  absorption, but also of absorptions due to isolated  $\text{NO}_2^-$  and to  $\text{Na}_x^+\text{NO}_2^-$ .

**12416.** Moore, G. A., **Design of a practical scanner unit for precision analysis of micrographs**, *Pattern Recognition* **3**, 91-122 (Oct. 1971).

**Key words:** Analysis of microstructures; automatic scanning (of micrographs); precision scanning (of micrographs); quantitative microscopy.

A precision mechanical scanner has been constructed for the purpose of preparing digital transcriptions of micrographs for computer analysis, and of performing elementary analysis without resort to a computer. Design criteria include convenience of operation and precision sufficient to correctly record all of the real information in one micrographic field.

Performance data are included. An analysis is given of the precision which may be expected in estimating area and volume percentage of a phase under various conditions. The attained precision is at least an order of magnitude greater than is normally obtained by manual methods.

**12417.** Post, M. A., **Copolymer determination in surface filler**, *Paint Varnish Prod.* **61**, No. 9, 31-38 (Sept. 1971).

**Key words:** Absorbance ratio method; infrared spectroscopy; resins; styrene-butadiene; surface fillers; vinyl toluene-acrylate; vinyl toluene-butadiene.

Styrene-butadiene, vinyl toluene-butadiene and vinyl toluene-acrylate copolymers in surface fillers are quantitatively determined by two methods. In one, a dual extraction method, which should be useful in acceptance testing of solvent type fillers, the

resin is determined as the difference between the total benzene and n-pentane extractables. The second method, a combination of single extraction and infrared analysis, involves determination of the total benzene extractables and the resin content therein. The latter is determined by measuring the 3.3  $\mu\text{m}/3.5 \mu\text{m}$  absorbance ratio of cast films from the benzene extract, using the baseline method, and reading the weight percent resin from the appropriate standard curve. This method depends on a constant ratio of styrene to butadiene, vinyl toluene to butadiene or vinyl toluene to acrylate. Its use is restricted to resins of a particular monomer ratio for which a standard curve has been made. These methods were developed and confirmed using commercially prepared fillers of known resin content.

**12418.** Prince, E., **Refinement of the crystal structure of apophyllite. III. Determination of the hydrogen positions by neutron diffraction**, *Am. Mineralogist* **56**, 1243-1251 (July-Aug. 1971).

**Key words:** Apophyllite; fluoro silicate; hydrated minerals; hydrogen bonds; mineral structure; neutron diffraction.

The crystal structure of apophyllite, a mineral with the ideal formula  $\text{KCa}_4(\text{Si}_4\text{O}_{10})_2\text{F} \cdot 8\text{H}_2\text{O}$ , has been refined using three-dimensional neutron diffraction data. 671 independent reflections were observed on a 4-circle diffractometer. Of these 516 had observable intensities. A least-squares refinement, with anisotropic temperature factors, led to an  $R$  index of 0.046. However, a difference Fourier synthesis revealed a region of negative scattering density in the vicinity of the fluorine atom. Accordingly a further refinement was carried out assuming a model in which 1/8 of the water molecules are replaced by  $\text{OH}^-$  ions, with the remaining proton bonded to fluorine to form an HF molecule. This model refined quickly to an  $R$  value of 0.037. The water molecules and OH ions are hydrogen bonded to the silicate framework. A preliminary mass spectrometric analysis of the gases evolved when apophyllite is heated revealed that the higher temperature specific-heat anomaly is due to the evolution of hydrogen fluoride. This suggests that the structural formula is  $\text{KCa}_4(\text{Si}_4\text{O}_{10})_2\text{F}_{1-x}(\text{HF})_x \cdot [(\text{H}_2\text{O})_{8-x}(\text{OH})_x]$  with  $x \approx 1$ .

**12419.** Scheer, M. D., Klein, R., McKinley, J. D., **Surface lifetimes of alkali metals on molybdenum**, *J. Chem. Phys.* **55**, No. 7, 3577-3584 (Oct. 1, 1971).

**Key words:** Alkali atoms; desorption energies; modulated beam method; polycrystalline molybdenum; surface ionization; surface lifetimes.

The surface lifetimes ( $\bar{\tau}$ ) of all the alkali metals on a polycrystalline molybdenum surface in the temperature region 900–1350 K were measured. The temperature dependence followed an Arrhenius expression of the form  $\bar{\tau}^\circ \exp(\bar{E}/kT)$ . Desorption energies ( $\bar{E}$ ) were found to be 3.14, 2.60, 2.53, 2.31, and 2.10 eV for Li, Na, K, Rb, and Cs. The corresponding pre-exponential factors ( $\bar{\tau}^\circ$ ) were  $3 \times 10^{-16}$ ,  $3 \times 10^{-15}$ ,  $2 \times 10^{-14}$ ,  $1 \times 10^{-13}$ , and  $3 \times 10^{-13}$  sec. From these data, ion and neutral desorption energies were calculated using a model employing a partial surface charge for the adsorbed particle and the Schottky relation. The validity of the Schottky relation for an adsorbed alkali was supported by analysis of recently available theory of partial charges. An explanation of the variation of the pre-exponential factors is presented on the basis of relative mobility of the adsorbed species. A pre-exponential factor was calculated using a partition function for an adsorbate with mixed localized and non-localized character. The extremes of completely localized and completely nonlocalized adsorption led to pre-exponentials that spanned the experimental values.

**12420.** Sher, A. H., Croll, W. K., Thurber, W. R., **Determination of oxygen in germanium below 20 parts per billion by measure-**

ments of lithium mobility and precipitation, *Anal. Chem.* **43**, No. 13, 1831-1834 (Nov. 1971).

Key words: Ge(Li) detectors; germanium; infrared absorption; lithium mobility; lithium precipitation; oxygen concentration.

The range of sensitivity and the expected degree of precision for the analysis of oxygen concentration in germanium by measurements of lithium-ion drift mobility and lithium precipitation have been determined. The relative sample standard deviations have been found to be  $\pm 10\%$  and  $\pm 15\%$ , respectively, in the range of oxygen concentration from 20 ppb (atomic) to 0.2 ppb (atomic). However, the lithium precipitation method alone cannot be used unambiguously in the determination of oxygen concentration in germanium. The sole previously-published value for the dissociation constant of the  $\text{LiO}^+$  complex in germanium at 295 K has been confirmed. A newly-observed feature in the lithium precipitation curve is shown to give semiquantitative information about oxygen concentration.

**12421.** Sher, A. H., Thurber, W. R., **Minority carrier and lithium-ion drift mobilities and oxygen concentration in *p*-type germanium**, *J. Appl. Phys.* **42**, No. 11, 4508-4509 (Oct. 1971).

Key words: Electron drift mobility; germanium diode; lithium-ion drift mobility; lithium precipitation; oxygen concentration; *p*-type germanium.

No correlations have been experimentally observed between electron drift mobility and lithium drift mobility nor between electron drift mobility and oxygen concentration in *p*-type germanium single crystals, as had been previously suggested.

**12422.** Shirk, J. S., **Laser excited fluorescence of  $\text{CCl}_2$** , *J. Chem. Phys.* **55**, No. 7, 3608-3609 (Oct. 1, 1971).

Key words: Fluorescence; force field; matrix.

Laser-excited fluorescence of  $\text{CCl}_2$  trapped in a low temperature matrix was observed in the 6000-8500 Å region. A normal coordinate analysis was carried out, using a Urey-Bradley force field, to determine the molecular force constants.

**12423.** Simpson, J. A., **Use of a microscope as a noncontacting microdisplacement measurement device**, *Rev. Sci. Instr.* **42**, No. 9, 1378-1380 (Sept. 1971).

Key words: Dimensional metrology; displacement measurement; microscope; noncontact sensing; optical surface probe; surface detection.

It is shown that a common research microscope with vertical illuminator can be easily converted to noncontacting measuring device of submicroinch resolution.

**12424.** Smith, S. J., **Molecular negative ion structure**, *Comments At. Mol. Phys.* **2**, No. 6, 175-180 (Feb.-Mar. 1971).

Key words: Elastic scattering; electron affinity; high resolution; internuclear distance; molecular negative ions; photodetachment.

This paper is a commentary on the reasons for limited progress in obtaining mechanical constants for molecular negative ions. It points out that two experimental technologies, one a sophistication of the photodetachment technique which incorporates energy analysis of detached electrons, the other a refinement of electron-neutral molecule scattering measurements with high energy resolution, now are yielding complementary data on molecular negative ion constants. In principle, these methods are widely applicable.

**12425.** Thomas, D. B., **Some studies on the reproducibility of tungsten-rhenium type thermocouples**, *Proc. 26th Intern. In-*

*strument Society of America Conf. and Exhibit on Advances in Instrumentation, Chicago, Ill., Oct. 4-7, 1971*, **26**, Part II, Paper 71-611 (Oct. 1971).

Key words: Anneal; argon; beryllium-oxide; calibrations; emf; helium; thermal-cycling; thermocouple; tungsten-rhenium; vacuum.

Representative samples of commercially available tungsten-rhenium type thermocouples were obtained from American manufacturers and calibrated in an argon atmosphere up to 2100 °C. After the initial calibrations were performed, the thermocouples were subjected to thermal-cycling between 1000 and 2100 °C and were also annealed for periods up to 420 hours at 2300 °C in argon. A comparison is made between the emfs of the thermocouples before and after the thermal-cycling and annealing periods. In general, the tungsten versus tungsten-26% rhenium thermocouples indicated the largest changes in emf after the thermal cycling and annealing periods while the tungsten-3% rhenium versus tungsten-25% rhenium thermocouples indicated the least change in emf. Some of the thermocouples were calibrated with and without beryllium-oxide insulation in argon, helium, and vacuum and a comparison is made between the thermocouple emfs under these conditions.

**12426.** Tsai, D. H., MacDonald, R. A., **Molecular dynamical studies of the phase transformation of iron under pressure**, (*Proc. Symp. Mechanisms of the Phase Transitions, University of South Carolina, Columbia, S.C., Feb. 1, 1971*), *Trans. Am. Crystallogr. Assoc.* **7**, 107-129 (Feb. 1, 1971).

Key words: Iron; lattice structure; martensitic transformation; molecular dynamics; phase diagram; P-V-T data.

We have applied molecular dynamics to the study of the transformation of iron from the  $\alpha$  phase (bcc) to the  $\epsilon$  phase (hcp) under hydrostatic pressure. The atomic interaction energy in both phases was represented by a two-body, central-force potential fitted (1) to the elastic properties of the  $\alpha$  phase at zero pressure and zero absolute temperature, and (2) to an assumed transition pressure of 130 kb at zero absolute temperature, with a volume decrease of 0.2 cm<sup>3</sup>/mol upon transition from the  $\alpha$  to the  $\epsilon$  phase. The classical equations of motion of the lattice points were solved by numerical computation, and the equation of state and specific heat data were obtained from the appropriate time-averages of the dynamical solutions. From these quantities, the Gibbs free energies of the two phases were calculated and a phase diagram for the  $\alpha$  to  $\epsilon$  transition was constructed. We found that the phase diagram thus obtained was in satisfactory agreement with experimental results. By observing the details of the lattice point motion given by the dynamical solutions, it was possible to follow the process of phase transformation when it occurred in the model. We describe here a martensitic type of buckling mechanism which was observed to transform the  $\alpha$  phase to the  $\epsilon$  phase.

**12427.** Tsang, W., Wasik, S. P., **The application of the isotope dilution GLC technique to air pollution analysis**, *J. Chromatog. Sci.* **9**, 567-569 (Sept. 1971).

Key words: Air pollution; benzene; benzene- $d_6$ ; gas analysis; gas chromatography; isotope dilution; sampling.

It is shown that the isotope dilution technique provides a simple means of accurately determining air pollutant concentrations under adverse conditions. This is demonstrated in various simulated situations with a sample of approximately 20 ppm benzene in argon.

**12428.** Wagner, H. L., Hoeve, C. A. J., **Effect of molecular weight on the refractive increment of polyethylene and *n*-alkanes**, *J. Polymer Sci.* **9**, Part A-2, 1763-1776 (1971).



**Key words:** Differential refractive index; differential refractometer; Lorentz-Lorenz; molecular weight; *n*-alkanes; polyethylene; polystyrene.

As in the case with other polymers previously reported, the values of the refractive index increment  $dn/dc$  of polyethylene and the *n*-alkanes change with molecular weight. Most of the variation may be understood by examination of the role of density in the Lorentz-Lorenz mixing equation of specific refractivity,  $R_{12} = \rho_1 R_1 + \rho_2 R_2$  used to calculate  $dn/dc$ . It may also be shown that as the absolute refractive index difference between solute and solvent becomes smaller,  $dn/dc$  becomes more sensitive to density change of the solute.

**12429.** Weir, C. E., **Concerning the maximum melting point**, *Japanese J. Appl. Phys.* **10**, No. 6, 714-716 (June 1971).

**Key words:** High pressure; melting point.

The theory of Kawai and Inokuti of the behavior of the melting point of solids as a function of pressure is discussed. The general theory is not considered applicable to the vast majority of materials known to date.

**12430.** Wexler, A., **Book review on "Modern Hygrometry"** by A. Pande, *Bull. Am. Meteorol. Soc.* **52**, No. 9, 897-898 (Sept. 1971).

**Key words:** Humidity; hygrometry; moisture; water vapor.

Book review on a monograph on the subject of hygrometry.

**12431.** Argentar, H., **Determination of the degree of polymerization of a polymeric amine from NMR data using a "least-squares" approach**, *J. Polymer Sci.* **9**, Part B, 657-659 (1971).

**Key words:** Aromatic amine; multiple regression analysis; nuclear magnetic resonance; polymer; proton magnetic resonance; spectroscopy.

A polymeric amine, the reaction product of 3,5-xylydine and the diglycidyl ether of bisphenol A, which had been synthesized and reported elsewhere, was analyzed by nuclear magnetic resonance spectroscopy (NMR). A statistical method was derived to estimate the degree of polymerization based on linear multiple regression analysis of the intensity of the NMR absorption peaks.

**12432.** Barnes, I. L., Sappenfield, K. M., Shields, W. R., **The mass spectrometric analysis of subpicogram quantities of lead**, (Proc. Int. Conf. Mass Spectroscopy, Kyoto, Japan, 1970), Chapter in *Recent Developments in Mass Spectroscopy*, K. Ogata and T. Hayakawa, eds., pp. 682-687 (University of Tokyo Press, Tokyo, Japan, 1970).

**Key words:** Lead; mass spectrometer; microsample.

An analytical method has been developed which gives stable measurable ion beams from samples containing  $10^{-8}$  to  $10^{-14}$  grams of lead.

Using a two stage twelve inch radius mass spectrometer equipped with an ion multiplier and electronics for fast pulse counting, a series of chemical microstandards loaded with known quantities of NBS standard lead samples (as small as  $10^{-14}$  grams of lead) were analyzed. These analyses showed that accuracy and precision of better than 0.5 percent (95% L. E. for a single analyses) could be obtained and that usually, the accuracy and precision were limited only by random counting statistics.

A series of quantitative analyses were done with two microgram or smaller samples taken from a single wafer of a silicate glass of known composition by the method of isotopic dilution. The required "spiking" of the sample was done utilizing an NBS Microstandard Ion Exchange Bead loaded with lead of known weight and composition.

The results obtained show severe cross-sectional variations of lead in the sample and demonstrate the importance of careful handling of samples for trace element analysis.

The use of the technique for the direct analyses of small crystals and/or particles is described. In this use only minimal chemical treatment is necessary thus eliminating most, if not all, of the usual sources of contamination and all chemical treatment may be performed directly on the mass spectrometer filament.

**12433.** Bederson, B., Kieffer, L. J., **Total electron-atom collision cross sections at low energies—A critical review**, *Rev. Mod. Phys.* **43**, No. 4, 601-641 (Oct. 1971).

**Key words:** Critical review; cross section measurement; electron-atom collisions; total cross section data.

Experiments relating to measurements of total and momentum-transfer cross sections for the scattering of low-energy electrons by atoms and diatomic molecules are critically reviewed. Principal emphasis is placed upon the Ramsauer method, dc swarms, and crossed-beams experiments, which account for the bulk of the reliable data in the literature although other techniques including differential measurements are also discussed. The theories of the various methods and possible sources of error are discussed. The case of low-energy electron scattering by helium is exhaustively reviewed since this system has been most intensively studied experimentally and is particularly amenable as well to theoretical calculations. The best available cross section values, along with comments on individual experiments, are presented in several tables.

**12434.** Bennett, L. H., Carter, G. C., **Enhanced lever rule for high-precision phase diagram determination**, *Met. Trans.* **2**, 3079-3081 (Nov. 1971).

**Key words:** Alloys; high precision; lever rule; nuclear magnetic resonance; phase diagrams.

A description is given of the conditions under which high-precision phase boundary determinations result from the application of the lever rule. This high precision results from a multiplication factor to the lever rule ratio, which is present only for experiments sampling one elemental site at a time. The multiplication factor is larger for smaller solubility limits. Precision of tenths of a percent can be readily attained under the indicated conditions. An example involving the  $^{115}\text{In}$  nuclear magnetic resonance for the determination of the solubility of  $\text{AuIn}_2$  in  $\text{AuAl}_2$  is presented.

**12435.** Blandford, J. M., Bensing, P. L., **Part I. Testing programs for the apparel industry. Part II. Evaluation of material and components**, Part I, 35 pages; Part II, 249 pages (2d ed.) (Apparel Research Foundation, Inc., Washington, D.C., May 15, 1971).

**Key words:** Apparel industry; equipment, textile testing; industry, apparel; performance, apparel materials; properties, apparel; quality control, apparel industry; test methods, textile; testing programs, apparel industry; textile testing, apparel materials.

This publication presents the details of minimum, intermediate, and advanced textile testing programs for evaluating the appearance and performance of materials and components used by the apparel industries. Tabulations give testing equipment, properties its use may determine, testing procedures and evaluation materials employed, and sources of supply and approximate prices of the equipment and evaluation materials.

Included are: (1) sections on the significance of a textile testing program, conditioning for testing textiles, performance requirements for textile fabrics, (American National Standard

L22), evaluation of fabric defects, and the availability of short laboratory training courses for apparel company employees; (2) bibliography; (3) reprints of the sixty-eight referenced test methods.

- 12436.** Brady, R. F., Jr., **Enolization of hexodiulose acetals. Synthesis of derivatives of D-psicose by reduction of a hex-3-enulopyranose**, *Carbohydrate Res.* **20**, 170-175 (Nov. 1971).

**Key words:** Cyclic acetals; hex-3-enulopyranose; hexodiulose; hexulose; psicose; stereospecific reduction; tagatose.

Previous papers from this laboratory have reported the synthesis of isopropylidene acetals of D-erythro-pentulose, D-threo-pentulose, D-fructose, and D-psicose, and have demonstrated their utility in the synthesis and purification of rare ketoses. The present work describes an attempt to synthesize similar acetals of D-tagatose (D-lyxo-hexulose). 1,2:4,5-Di-O-isopropylidene- $\beta$ -D-erythro-2,3-hexodiulo-2,6-pyranose (1), an intermediate previously used, was converted into a 3,4-enediol acetate, namely, 1,2:4,5-di-O-isopropylidene- $\beta$ -D-glycero-hex-3-enulopyranose (2). Reduction of 2 with hydrogen over palladium gave, however, only 3-O-acetyl-1,2:4,5-di-O-isopropylidene- $\beta$ -D-psicopyranose (3), and none of the D-tagatose derivative.

The synthesis and synthetic applications of fully protected aldoses and diuloses have received much attention, but the chemistry of enediol acetates, as obtained from these compounds by the action of acetic anhydride-triethylamine, is largely unexplored. Stereospecific reduction or addition reactions of these unsaturated derivatives offer attractive possibilities for the synthesis of rare and unusual sugars.

- 12437.** Brauer, G. M., **A review of recent studies of in vitro reactivity of surfaces of calcified tissues**, (Proc. Int. Symp. Calcified Tissues, Dental and Surgical Materials and Tissue Material Interactions, University of Nijmegen, Nijmegen, The Netherlands, 1970), *Dent. Tissues Mater.*, pp. 193-231 (1971).

**Key words:** Adhesion to tooth surfaces; adsorption on calcified tissues; bone; calcified tissues; dentin; enamel; modification of tooth surfaces; reactivity of calcified tissues.

Studies of the reactivity and modification of tooth surfaces offer an attractive approach for obtaining useful information to reduce dental caries and improve adhesion between tooth structure and restoratives. Investigation of the interaction of gases on such surfaces provides considerable insight into the structural details of surfaces of hard tissues. Effectiveness of potential conditioning agents can be demonstrated from alterations of the surface properties of teeth as indicated by changes in: critical surface tension, oil-wettability, adsorption isotherms and adhesionability. Measurement and evaluation of heats of immersion and heats of reaction are useful for observing modifications and determining those groups that bond to tooth structure in aqueous environments. Application of dilute polyfunctional acids removes debris, etches enamel and increases surface wettability. Etching creates an increased surface area and opens pores into which resin can flow. Excellent adhesion is obtained after hardening because of mechanical interlocking of resin at the enamel-resin interphase. Long side chains have been grafted to collagenous surfaces (collagen powder or film, bone). Grafting monomers containing additional functional groups that are potential reactive centers for further modification is feasible. Surfaces with the desired degree of hydrophil-lipophil balance to suit specific applications can be prepared.

- 12438.** Brown, W. E., **Physicochemical aspects of decay and decalcification**, (Proc. Int. Symp. Calcified Tissues, Dental and Surgical Materials and Tissue Material Interactions, University of Nijmegen, Nijmegen, The Netherlands, 1970), *Dent. Tissues Mater.*, pp. 69-97 (1971).

**Key words:** Calcium phosphate; caries; caries mechanism; enamel; hydroxyapatite; tooth mineral; solubility.

Much of the research directed toward understanding the "mechanism" of dental caries has been etiological in nature and has delineated the importance of certain micro-organisms and their products in producing caries. However, attempts to provide physicochemical models have been few in number, and because of the complexity of the system and lack of knowledge about some of the most important parameters, these models have been relatively primitive. Our increasing knowledge about the character of carious lesions, enamel surfaces, and plaque now make such a model more attainable. The purpose of such a model is not to describe quantitatively the caries process, *per se*, but instead to identify the essential or rate controlling steps that can then be modified to prevent caries.

The objective of this paper is to provide a thermodynamic and kinetic basis for developing such models. The phase diagrams for calcium phosphates in ternary and more complex systems are shown to be an essential basis and they have important implications regarding (1) the observation that  $\beta$ -Ca<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub> is found in the carious lesion, and (2) the possible significance of variations in the solubility of the mineral phase relative to caries susceptibility. Transport mechanisms may prove to be crucial to the formation of caries, particularly when coupled with the fact that the isotherms for calcium phosphates have positive slopes in the (Ca) vs. (P) solubility diagrams. A model intermediate to the Donnan-membrane and the strictly diffusional types may prove to be the most appropriate.

- 12439.** Burdick, M. D., **A test for the cleanability of surfaces finishes**, *Porcelain Enamel Inst. Bull.* **T-28**, pp. 1-17 (1971).

**Key words:** Cleanability; fluorescence; porcelain enamel.

A detailed procedure is given to permit a numerical evaluation of the cleanability of surfaces. The method employs a fluorescent, water soluble soiling agent, a mechanized procedure for its application and partial removal, the water extraction of the retained soil and the calculation of a cleanability index through the use of a standard reference surface.

- 12440.** Casella, R. C., **The reversal symmetry and its breaking in physics**, *Phys. Teacher* **8**, No. 3, 114-123 (Mar. 1970).

**Key words:** CPT; K<sup>0</sup> meson; symmetry; time-reversal; weak decays.

A review of symmetry principles in physics including charge conjugation (C), parity (P), and time reversal (T) is given, with emphasis on T symmetry and its breaking in K<sup>0</sup> meson decay. Following the 1956 discovery of P violation, CP, T, and CPT were assumed valid. The discovery in 1964 of CP breaking in K<sup>0</sup> decay into pions coupled with the CPT theorem implies T violation there, but T symmetry remains intact in several closely related experiments, suggesting the need for a direct demonstration of T violation. An account is included of the author's analysis which provides this demonstration.

- 12441.** Cooper, M. J., **Generalized scaling and the parametric equation of state in the critical region**, Chapter in *Critical Phenomena in Alloys, Magnets, and Superconductors*, pp. 77-87 (McGraw-Hill Book Co., Inc., New York, N.Y., 1971).

**Key words:** Critical phenomena; equation of state; parametric equation of state; scaling laws.

A description of the critical region is developed using a local parametric characterization of the thermodynamic potential surface. The physical consequences of the formalism are presented and its predictions compared with some of the experimental data. Results indicate an extended description of the thermodynamic properties over a much enlarged region about the critical point.



**12442.** Corliss, E. L. R., Estimate of the inherent channel capacity of the ear, *J. Acoust. Soc. Am.* **50**, No. 2, 671-677 (1971).

Key words: Articulation function of ear; "bit" capacity of ear; channel capacity of ear; distinctive features of ear and hearing; intelligibility vs word lengths as block codes; speech; word lengths as block codes; speech intelligibility as channel capacity.

The growth of intelligibility of speech stimuli as a function of level above hearing threshold can be computed from the "circuit parameters" of the hearing mechanism by applying Shannon's concepts of channel capacity, equivocation, and "bits." In the ear, the unit response is an effective "least count," derived from experimental data on hearing by means of the equations for a model resembling a frequency-selective circuit [E. Corliss, *J. Acoust. Soc. Amer.* **41**, 1500-1516 (1967)]. The model predicts that the number of least counts available rises as the one-fourth power of the signal intensity above threshold. Experimentally, this growth rate is observed for the intensity-resolving power of the ear. Approximately the same power law is observed for the sensation of loudness. The model ascribes both effects to the same mechanism. From the observed integration time of the ear, the model predicts the rate at which transitions of single counts can be detected. From the counting rate and the integration time, the channel capacity available at the ear and its increase with level above the threshold can be computed. The information content of speech as a source function is evaluated from the rate at which single "distinctive features" of speech phonemes are produced. Intelligibility scores can be predicted from the ratio between the rate at which information is being produced by the source and the rate at which the receptor can accept the source material. The scores predicted agree fairly closely with experimental data on random-word and random-syllable intelligibilities. This agreement shows that the listener need recognize no more than a single distinctive feature of each phoneme to display the recognition functions that have been observed. From a theorem of C. Shannon [Inform. and Control **1**, 6-25 (1957)] relating code length and error probability, one can show that the channel capacity required for polysyllabic words is lower than the channel capacity required for monosyllabic words because the duration of correlated utterance may be taken as a code length. Evidently, contextual effects are not prominent in the intelligibility of random-word lists; the hearing process involved is primarily recognition of groups of sounds; meaning is secondary. The results also lead to the inference that a direct relation may exist between channel capacity and perceived loudness when speech is transmitted over a broad-band system, and suggest that loudness functions for impaired ears might prove to be correlated with intelligibility functions.

**12443.** Coxon, B., Studies of  $^{15}\text{N}$ -labeled amino sugars. The synthesis and mass spectrometry of derivatives of 6-amino-6-deoxy-D-glucose- $^{15}\text{N}$ , *Carbohydrate Res.* **19**, 197-210 (1971).

Key words: Derivatives of 6-amino-6-deoxy-D-glucose- $^{15}\text{N}$ ; differential scanning calorimetry; infrared isotopic shift; mass spectrometry; nucleophilic substitution;  $^{15}\text{N}$ -labeled amino sugars;  $^{15}\text{N}$ -trifluoroacetyl derivative.

Derivatives of 6-amino-6-deoxy-D-glucose- $^{15}\text{N}$  have been synthesized in high yield and high chemical and isotopic purity by reaction of the 6-*O*-*p*-tolylsulfonyl or 6-deoxy-6-iodo derivative of 1,2:3,5-di-*O*-isopropylidene- $\alpha$ -D-glucopyranose with potassium phthalimide- $^{15}\text{N}$ . The infrared and mass spectra of some of these derivatives are discussed. Comparisons of the mass spectra of the  $^{14}\text{N}$  compounds and  $^{15}\text{N}$ -labeled derivatives afforded confirmation of the pathways of fragmentation.

**12444.** Coxon, B., Johnson, L. F., The N.M.R. spectroscopy of derivatives of 6-amino-6-deoxy-D-glucose- $^{15}\text{N}$ .  $^{13}\text{C}$  Fourier-

transform and internuclear, double- and triple-resonance studies, *Carbohydrate Res.* **20**, 105-122 (Nov. 1971).

Key words: Internuclear double resonance; internuclear triple resonance; nitrogen-15 coupling constants; nuclear Overhauser effects; p.m.r. spectroscopy; 6-amino-6-deoxy-D-glucose- $^{15}\text{N}$  derivatives;  $^{13}\text{C}$  n.m.r. spectroscopy;  $^{15}\text{N}$  n.m.r. spectroscopy.

A series of  $^{15}\text{N}$ -labeled 6-amino-6-deoxy-1,2:3,5-di-*O*-isopropylidene- $\alpha$ -D-glucopyranose derivatives and their  $^{14}\text{N}$  analogs has been studied by continuous-wave proton,  $^{13}\text{C}$ , and  $^{19}\text{F}$  magnetic resonance spectroscopy, and by  $^{13}\text{C}$  Fourier-transform techniques. Characteristic chemical shifts and the magnitudes of  $^1\text{H}$ - $^1\text{H}$ ,  $^1\text{H}$ - $^{15}\text{N}$ ,  $^1\text{H}$ - $^{19}\text{F}$ ,  $^{13}\text{C}$ - $^{15}\text{N}$ , and  $^{15}\text{N}$ - $^{19}\text{F}$  coupling-constants are reported and discussed. The  $^1\text{H}$ - $^{15}\text{N}$  and  $^{13}\text{C}$ - $^{15}\text{N}$  coupling-constants over one bond have been used to assess the hybridization of the  $^{15}\text{N}$  atom in three of the derivatives. Heteronuclear, internuclear, double-resonance (indor) and triple-resonance ("intripler") experiments have been performed in which  $^{15}\text{NH}$  proton transitions were monitored while the  $^{15}\text{N}$  or  $^{19}\text{F}$  frequencies were swept or maintained on resonance. Replicas of the computed, theoretical  $^{15}\text{N}$  spectrum were recorded indirectly, and are discussed in relation to nuclear Overhauser effects.

**12445.** Davis, J. E., The dry and wet bulb psychrometer, (Proc. ASHRAE Symp. Humidity Measurement, Columbus, Ohio, Feb. 5-8, 1968), Chapter in *ASHRAE (Amer. Soc. Heat. Refrig. Air-Cond. Eng.) Bull. Humidity Measurement*, pp. 6-17 (May 1970).

Key words: Aspiring psychrometers; dry- and wet-bulb psychrometers; errors in psychrometric measurements; psychrometric formulas; thermocouple psychrometers; thermodynamic wet bulb temperature.

A paper describing the state of the art of dry and wet bulb psychrometry is presented. Mathematical relationships applicable to a sling psychrometer (or a dry and wet bulb thermometer in a test duct) are given. Short discussions of the universal psychrometric formula and three equations for use with the sling psychrometer are presented. Two of these equations consider effects which cause the reading of the wet-bulb to deviate from the true thermodynamic wet bulb temperature, but they have limitations which are described. The aspiring psychrometer is discussed and the performance of a simple thermocouple psychrometer devised at the National Bureau of Standards is described. Accuracy, precision, and laboratory fabrication techniques are also discussed. Results of tests at NBS using techniques published by earlier investigators at temperatures at 32 °F (0 °C) or below are given. Reference is made to instruments developed which measure true thermodynamic wet bulb temperature, but in their present stage of development are too large to be used in a test duct.

**12446.** Dibeler, V. H., Walker, J. A., McCulloh, K. E., Rosenstock, H. M., Effect of hot bands on the ionization threshold of some diatomic halogen molecules, *Intern. J. Mass Spectrom. Ion Phys.* **7**, 209-219 (1971).

Key words: Halogen molecules; hot bands; ionization threshold; mass spectrometry; monochromator; vacuum ultraviolet.

Photoion-yield curves are obtained for the molecular ions of the homonuclear diatomic halogens and for iodine monochloride and iodine monobromide. Excepting iodine, ionization thresholds of ground-state and vibrationally-excited molecules are separately identified by measurements made at several ion-source temperatures. The adiabatic ionization energies (in eV) are:  $I(\text{F}_2) = 15.69$ ,  $I(\text{Cl}_2) = 11.48$ ,  $I(\text{Br}_2) = 10.52$ ,  $I(\text{I}_2) = 10.07$ ,

and  $I(\text{I}^+)=9.79$ . A preferred value of  $I(\text{I}_2)=9.37$  eV is proposed.

**12447.** DiMarzio, E. A., Rubin, R. J., **Adsorption of a chain polymer between two plates**, *J. Chem. Phys.* **55**, No. 9, 4318-4336 (Nov. 1, 1971).

Key words: Adhesion; grand canonical ensemble formalism; polymer adsorption; random walk model.

A lattice model of adsorption of an isolated chain polymer between two plates is investigated using a matrix formalism and a grand canonical ensemble (GCE) formalism. The matrix formalism is particularly convenient for calculating the polymer segment density as a function of the distance from one of the plates for different fixed plate separations. The GCE formalism can be used to calculate the fraction of loops (sequences of polymer segments whose ends are in contact with one plate and whose intermediate segments lie between the two plates), bridges (sequences of polymer segments whose ends are in contact with different plates and whose intermediate segments lie between the two plates), and trains (sequences of polymer segments which are wholly in contact with one plate or the other). All of the foregoing quantities have been calculated in the limit of infinite molecular weight as a function of the distance of separation between the plates and the energy of adsorption of a polymer segment on a plate. The self-excluded volume of the polymer chain is ignored. In addition the average sizes of loops, bridges, and trains, and the effective force of attraction between the plates are calculated.

**12448.** Distefano, G., Dibeler, V. H., **Photoionization study of the dimethyl compounds of zinc, cadmium, and mercury**, *Intern. J. Mass Spectrom. Ion Phys.* **4**, 59-68 (1970).

Key words: Heats of formation; ionization thresholds; mass spectrometry; metal alkyls; photoionization.

Photoionization yield curves from onset to 600 Å and ionization threshold values have been obtained for the ions  $\text{M}(\text{CH}_3)_2^+$ ,  $\text{CH}_3\text{M}^+$  and  $\text{M}^+$  of the dimethyl compounds of zinc, cadmium, and mercury, and the  $\text{CH}_3^+$  from dimethyl-mercury. Bond dissociation energies and heats of formation of the ions are also reported.

**12449.** Durst, R. A., **Ion-selective electrodes in science, medicine, and technology**, *Am. Sci.* **59**, No. 3, 353-361 (May-June 1971).

Key words: Electrodes; ion-selective electrodes; ion-selective electrode review; membrane electrodes; potentiometry.

The state of the art of the newer, non-glass types of ion-selective electrodes is reviewed. This brief survey includes discussions of the characteristics of the solid-state, liquid ion-exchange, and heterogeneous membrane electrodes. Applications of these sensors to a wide variety of scientific disciplines is presented, including biomedical research and industrial monitoring and control systems.

**12450.** Fatiadi, A. J., **(p-Bromophenyl)osotriazoles from inositols**, *Carbohydrate Res.* **20**, 179-184 (Nov. 1971).

Key words: Infrared; inositol; osotriazole; parabromophenyl; preparation; spectra; study.

(p-Bromophenyl)osotriazoles from inositols ( $\text{D}_1\text{L}$  and  $\text{DL}$ ), (+) proto-quercitol and their derivatives have been prepared and characterized. The KBr matrix i.r. spectra of  $\text{D}$ ,  $\text{L}$  and  $\text{DL}$  forms revealed some differences.

**12451.** Flynn, T. M., Smith, C. N., **Trends in cryogenic fluid production in the United States**, (Proc. Int. Institute of Refrigeration, Tokyo, Japan, 1970), *Int. Inst. Refrig. Bull. Suppl. Commission I*, pp. 241-247 (Annex 1970-2).

Key words: Argon; cryogenics; forecasts; helium; hydrogen; liquefied natural gas; nitrogen; oxygen; trends.

The cryogenic industry in the United States has changed dramatically in both scope and character during the last decade. It has progressed from a liquid hydrogen technology to a liquid helium technology to developing new technologies dependent upon both the upper and lower extremes of the cryogenic scale. Among these are practical applications of superconductivity and the use of liquefied natural gas as a major world energy source. This change in the nature of the industry, and some of its implications for the future, is seen in this paper which traces the production of the economically significant cryogenics over the last decade and gives the present status of cryogen in the U.S.A.

**12452.** Franklin, A. D., **Theory of linear dielectrics**, Chapter 17 in *Proc. Conf. Electronic Phenomena in Ceramics*, University of Florida, Gainesville, Fla., Nov. 10-14, 1969, pp. 451-489 (1971).

Key words: Ceramics; dielectric constant; electronic polarization; interfacial polarization; lattice polarization; orientation polarization; theory.

A cursory review is given of the theory of the linear response of a dielectric to an impressed electric field, including the electronic, lattice, dipole orientation, and linear interfacial polarizations. Most emphasis is given to the crystalline ionic, insulating models appropriate for the more ionic ceramics. Modifications to the theory for semiconducting and vitreous materials are briefly touched upon.

**12453.** Haar, L., Shenker, S. H., **Equation of state for dense gases**, *J. Chem. Phys.* **55**, No. 10, 4951-4958 (Nov. 15, 1971).

Key words: Argon; compressibility factor; dense fluids; equation of state; molecular dynamics; molecular interactions; nitrogen; pair potentials; temperature perturbation theory.

A simple quantitative equation of state of the van der Waals type is proposed for dense fluids. The equation yields compressibility factors with a precision comparable to those from the more complicated temperature perturbation theory when tested against "computer experiments," including isotherms as low as 0.8 liquid-vapor critical temperature. The equation is capable of predicting compressibility factors for real gases as illustrated by calculations for argon and nitrogen at pressures up to 10,000 atm. The derivation of the equation is based on a rearrangement of the terms in the Ursell-Mayer density expansion of the configuration integral. The equation contains two temperature-dependent parameters, to be determined from the dilute gas second virial coefficients. A principal feature of our approach is that it does not require explicit knowledge of the details of the pair interaction.

**12454.** Hall, J. L., Barger, R. L., Bender, P. L., Boyne, H. S., Faller, J. E., Ward, J., **Precision long path interferometry and the velocity of light**, A. Smolinski and S. Hahn, eds., (Proc. URSI Conf. Laser Measurements, Warsaw, Poland, Sept. 24-26, 1968), *Electron Technol.* **2**, No. 2/3, 53-66 (Panstwowe Wydawnictwo Naukowe Polish Scientific Publ., Warsaw, Poland, 1969).

Key words: Interferometry; laser; optical heterodyne; velocity of light.

A JILA/NASA/NBS velocity of light experiment has recently been started using the 51 Gc neon laser doublet at 1.15 microns. An evacuated 30-meter Fabry-Perot interferometer has been servo-stabilized to  $\sim 1:10^6$ .



**12455.** Hussmann, E. K., McLaughlin, W. L., **Dye films and gels for megarad dosimetry**, *Proc. United Kingdom Panel on Gamma and Electron Irradiation, The National Physical Laboratory, Teddington, England, July 1970*, pp. 35-60 (Apr. 1971).

**Key words:** Depth-dose dyes; dose distribution; dosimetry; electrons; films; gamma rays; gels; radiation beams; x rays.

Gel, liquid, and thin-film radiochromic dye systems developed by McLaughlin and Chalkley are shown to be useful for measuring large doses from electron and x- and gamma-irradiations. The thin films are particularly suited to imaging and measuring radiation field profiles and dose distributions in various materials, even across interfaces of media with different stopping powers and absorption coefficients.

**12456.** Johannesen, R. B., Duerst, R. W., **Nuclear magnetic resonance studies of inorganic fluorides. VI. Magnetic nonequivalence in bis(perfluorovinyl) mercury**, *J. Magn. Resonance* **5**, No. 3, 355-366 (Dec. 1971).

**Key words:** Double resonance; fluorine; INDOR; mercury; nuclear magnetic resonance.

Fluorine magnetic resonance and  $^{199}\text{F}\{^{199}\text{Hg}\}$  resonance spectra of bis(perfluorovinyl)mercury and methyl(perfluorovinyl)mercury have been observed. Proton resonance and  $^1\text{H}\{^{199}\text{Hg}\}$  spectra of methyl(perfluorovinyl)mercury and dimethylmercury have also been observed. The magnitudes and signs of all possible F—F, F—Hg, and H—Hg coupling constants in these three compounds have been determined. The spectrum of bis(perfluorovinyl)mercury calculated from the determined parameters is in excellent agreement with observation and the presence of long-range F—F coupling constants in this molecule, none of which are zero, verifies an earlier suggestion as to the reason for the complexity of the spectrum. The fluorine chemical shifts and F—F coupling constants within a perfluorovinyl group are within the previously reported range for these parameters. The mercury chemical shifts determined by INDOR spectroscopy are as follows: dimethylmercury 0 (reference), methyl(perfluorovinyl)mercury +  $482 \pm 3$  ppm, bis(perfluorovinyl)mercury +  $957 \pm 3$  ppm.

**12457.** Julienne, P. S., Krauss, M., Donn, B., **Formation of OH through inverse predissociation**, *Astrophys. J.* **170**, 65-70 (Nov. 15, 1971).

**Key words:** Interstellar clouds; interstellar molecule formation; inverse predissociation; non-adiabatic mixing; OH radiative association rate; predissociation widths.

Formation of OH can occur by inverse predissociation from continuum levels to the  $v=1$ ,  $k=1$  level of the  $A\ ^2\Sigma^+$  state. A rate constant of  $1 - 3 \times 10^{-20}$  cm<sup>3</sup> s<sup>-1</sup> is calculated for temperatures greater than 20 K. Predicted OH densities are consistent with observations in dense, heavily obscured clouds but appear to be somewhat low for H I clouds.

**12458.** Julienne, P. S., Neumann, D., Krauss, M., **Calculation of the temperature dependence for absorption in CO<sub>2</sub> in the 1750—1200 Å region**, *J. Atmospheric Sci.* **28**, No. 6, 833-837 (Sept. 1971).

**Key words:** *Ab initio* potential curve; carbon dioxide; quasi-linear molecule; Renner splitting; temperature dependent absorption coefficient; transition moment; ultraviolet.

The absorption cross section of the diffuse absorption bands of CO<sub>2</sub> in the region 1750—1200 Å is of prime importance for understanding CO<sub>2</sub> photolysis, especially as a constituent of a planetary atmosphere. The upper state of the absorption is a  $^1\text{B}_2$  state correlating with a  $^1\Delta_u$  state in the linear geometry. Although

the cross section for this vibronically allowed electric-dipole absorption will be temperature-dependent, there are no experimental studies of this temperature dependence, and room temperature values have been used in discussions of the atmospheres of Mars and Venus despite the widely disparate temperature distributions of their atmospheres.

We have calculated the temperature dependence of the integrated absorption coefficient for the 1750—1200 Å region. The electronic energies and transition moments were calculated *ab initio* as a function of the bending angle of the molecule; in this way the Renner type splitting of the degenerate  $^1\Delta_u$  state into  $^1\text{B}_2$  and  $^1\text{A}_2$  energy curves is obtained. The integrated absorption cross section is proportional to the square of the transition moment averaged over the ground state vibrational wave functions. At room temperature the average of the transition moment squared over a Boltzmann distribution is  $2.9 \times 10^{-3}$  (ea<sub>0</sub>)<sup>2</sup>, which corresponds roughly to an oscillator strength of  $6 \times 10^{-4}$ . Although halving the temperature produces only about 10% decrease in absorption, there is a dramatic increase by 75% when the temperature is doubled. The temperature dependence of individual lines, particularly in the wings of the overall distribution, is likely to be even more sensitive.

**12459.** Kaldor, A., **Absorption spectrum of borazine in the vacuum ultraviolet**, *J. Chem. Phys.* **55**, No. 9, 4641-4643 (Nov. 1, 1971).

**Key words:** Borazine; gas phase; matrix isolation; photochemistry; spectra; vacuum ultraviolet; vibronic structure.

The absorption spectrum of both vapor-phase and matrix-isolated borazine has been investigated in the 2000–1500-Å region. Three electronic transitions have been observed. The strongest absorption, with a maximum at 1650 Å, is assigned to the allowed  $^1E' - ^1A_1'$  transition. Two weaker absorptions, with forbidden origins at 1975 and 1889 Å, are assigned to the forbidden transitions  $^1A_2' - ^1A_1'$  and  $^1A_1' - ^1A_1'$ , respectively. The  $^1A_2' - ^1A_1'$  transition is made vibronically allowed by one quantum change in the  $\nu_{16}$  and  $\nu_{17} e'$  vibrations. The vibration making allowed the  $^1A_1' - ^1A_1'$  transition could not be determined.

**12460.** Kao, R., Perrone, N., Capps, W., **Large-deflection solution of the coaxial-ring-circular-glass-plate flexure problem**, *J. Am. Ceramic Soc.* **54**, No. 11, 566-571 (Nov. 1971).

**Key words:** Coaxial; deflection; flexure; glass; numerical; plate; ring; solution; strength; stress.

Nonlinear deflections and radial surface stresses in thin elastic circular plates laterally deformed into symmetrical concave shapes are analyzed. The deformations are induced by loading each plate with a small center ring while the plate is resting on a ring of nearly the same diameter as the plate. The rings and plate are coaxial, i.e., concentric. Center deflections up to 3 and 4.5 times the plate thickness were predicted for ring-diameter ratios of 0.5 and 0.2, respectively. The predicted deflection profiles at various loads agreed quite well with those which were determined experimentally on a chemically strengthened glass plate. This analysis provides a new criterion for using the coaxial-ring loading method for flexural strength of brittle materials.

**12461.** Kaufman, V., Sugar, J., **One-electron spectrum of doubly ionized lutetium (Lu III) and nuclear magnetic dipole moment of  $^{175}\text{Lu}$** , *J. Opt. Soc. Am.* **61**, No. 12, 1693-1698 (Dec. 1971).

**Key words:** Lutetium; spectra; wavelengths.

Thirteen new terms of the  $4f^{14}(^1S_0)nl$  doublet system of Lu<sup>2+</sup> have been found, comprising the *ns* series ( $7 \leq n \leq 10$ ), the *nf* series ( $5 \leq n \leq 9$ ), and the *5g*, *6d*, *7d*, and *7p* terms. Previously, only the *5d*, *6s*, and *6p* terms were known. The *ns* series was

used to derive an ionization energy of  $169049 \pm 10 \text{ cm}^{-1}$ . From the completely resolved hyperfine structure (hfs) of  $6s^2 S_{1/2}$ , the value  $a(6s) = 0.436 \pm 0.002 \text{ cm}^{-1}$  was obtained for the hyperfine splitting factor. With these data, the nuclear magnetic dipole moment  $\mu_I$  was found to be  $2.204 \pm 0.010 \mu_N$ , where the stated uncertainty includes only the experimental uncertainty for  $a(6s)$ .

**12462.** McBee, C. L., Kruger, J., **Optical changes in oxide films on iron prior to breakdown**, *Nature Phys. Sci.* **230**, No. 17, 194-195 (Apr. 26, 1971).

Key words: Chloride; ellipsometry; passive film; spectroscopy.

Evidence for optical changes in the passive film on iron prior to complete breakdown by chloride is presented. The technique of ellipsometric-spectroscopy is used to locate a wavelength affected by the chloride addition. The recovery of the passive film by removal of the chloride ion is also reported.

**12463.** McDowell, H., Brown, W. E., Sutter, J. R., **Solubility study of calcium hydrogen phosphate. Ion-pair formation**, *Inorg. Chem.* **10**, 1638-1643 (Aug. 1971).

Key words: Calcium-phosphate ion pairs; solubility of anhydrous dicalcium phosphate; solubility of calcium monohydrogen phosphate; solubility of dibasic calcium phosphate; solubility of dicalcium phosphates.

The solubility of  $\text{CaHPO}_4$  has been determined in the ternary system  $\text{Ca}(\text{OH})_2 - \text{H}_3\text{PO}_4 - \text{H}_2\text{O}$ , at 5, 15, 25, and  $37^\circ$ . The solubility product constant,  $K_{sp} = (\text{Ca}^{2+})(\text{HPO}_4^{2-})$ , varies with pH unless formation of ion pairs  $\text{CaHPO}_4^0$  and  $\text{CaH}_2\text{PO}_4^+$  is taken into consideration. Solubility product constants and their standard errors for  $\text{CaHPO}_4$  are  $(1.97 \pm 0.03) \times 10^{-7}$ ,  $(1.64 \pm 0.01) \times 10^{-7}$ ,  $(1.26 \pm 0.02) \times 10^{-7}$ , and  $(0.92 \pm 0.02) \times 10^{-7}$  at 5, 15, 25, and  $37^\circ$ , respectively. Association constants and standard errors are  $(2.4 \pm 0.3) \times 10^2$ ,  $(1.9 \pm 0.2) \times 10^2$ ,  $(3.8 \pm 0.5) \times 10^2$ , and  $(3.9 \pm 0.9) \times 10^2$  for  $\text{CaHPO}_4^0$  and  $5 \pm 1$ ,  $10 \pm 1$ ,  $10 \pm 1$ , and  $11 \pm 1$  for  $\text{CaH}_2\text{PO}_4^+$  at the same respective temperatures. Thermodynamic functions for the dissolution reaction for  $\text{CaHPO}_4$  and the association reactions for  $\text{CaHPO}_4^0$  and  $\text{CaH}_2\text{PO}_4^+$  are also presented.

**12464.** Martin, W. C., **Energy differences between two spectroscopic systems in neutral, singly ionized, and doubly ionized lanthanide atoms**, *J. Opt. Soc. Am.* **61**, No. 12, 1682-1686 (Dec. 1971).

Key words: Atomic spectra; electron configurations; energy levels; lanthanide elements; spectra.

Energy differences of the type  $4f^{N-1} 5d - 4f^N$  (doubly ionized atoms),  $4f^{N-1} 5d6s - 4f^N 6s$  (singly ionized atoms), and  $4f^{N-1} 5d6s^2 - 4f^N 6s^2$  (neutral atoms) are important for the interpretation of rare-earth spectra. Here  $N = 1$  for La, ... 14 for Yb, and each configuration is represented by its lowest level in these system differences (SD). Nineteen of these differences are now known exactly from analyses of the spectra. Five additional SD values are approximately fixed by a combination of observation and calculation. Regularities deduced from these known values allow predictions for the remaining 18 SD values. The estimated probable error for most of the predictions is either 1000 or 1500  $\text{cm}^{-1}$ .

**12465.** Masters, L. W., Lutz, G. J., **Determination of thallium by photon activation analysis**, *Anal. Chim. Acta* **56**, 365-370 (1971).

Key words: Activation analysis; bremsstrahlung; determination; glass; photon activation analysis; thallium.

The determination of trace amounts of thallium by the thermal neutron reaction  $^{203}\text{Tl}(n,\gamma) ^{204}\text{Tl}$  is complicated because  $^{204}\text{Tl}$  is a

pure beta-emitter, requiring a lengthy and rigorous separation. In addition the half-life of  $^{204}\text{Tl}$  is too long to permit decay measurements. A photon activation analysis method has been developed for this determination. Bremsstrahlung from a beam of 35-MeV electrons induces the photonuclear reaction  $^{203}\text{Tl}(\gamma,n) ^{204}\text{Tl}$ . The detection limit is of the order of tens of nanograms. It was determined that there are no interfering photonuclear reactions from lead.

**12466.** Moore, R. T., **Determination of performance of digital data communication systems**, (Proc. IEEE, ICC 71 CIC Intern. Conf. Communications, Montreal, Canada, June 14-16, 1971), IEEE, ICC 71 CIC Conf. Record VII, Session 12A, VIII, 12-1-12-3 (1971).

Key words: Digital data communication; digital system performance; draft standard ANSI X3; RER; TOT; TRIB.

An overview is presented of the work of American National Standards Institute Task Group X3S3.5 in the development of a standard for the determination of the performance of data communication systems.

Four performance criteria are identified. These are: (1) Transfer Rate of Information Bits (TRIB), a measure of information throughput; (2) Transfer Overhead Time (TOT), a measure of delays associated with the communications process; (3) Residual Error Rate (RER); and (4) System Availability (A). These criteria, as defined, are independent and are both necessary and sufficient to express the performance of any Information Path operated in accordance with the applicability limitations of the document.

Data communications system description is developed on a functional rather than a physical basis, and only to the extent necessary for performance determination.

The five possible phases of data communication are identified as: (1) Connection Establishment, (2) Link Establishment, (3) Information Transfer, (4) Link Termination, and (5) Connection Disestablishment. The beginning and end of each of these phases is rigorously defined and these definitions support the methodology for determining values for the performance criteria TRIB and TOT.

**12467.** Nagasawa, T., Kobayashi, K., **Paracrystalline structure of polymer-crystal lattice distortion induced by electron irradiation**, *J. Appl. Phys.* **41**, No. 11, 4276-4284 (Oct. 1970).

Key words: Crystal; defects; irradiation; polyethylene; unit cell.

The melting temperature of polyethylene crystals decreases and the lattice constants (both  $a$  and  $b$ ) and lattice distortion increase, but the macroscopic volume of the specimen does not change with electron irradiation. From these results a model of a deformed lattice structure with point defects produced by irradiation is proposed. Calculations indicate that the anisotropy of a polymer crystal (difference between the elastic modulus along the molecular axis and perpendicular to the axis) increases the range of the distortion in a crystal caused by a defect. The presence of lattice distortion in electron irradiated polymer single crystals produces observable features in the Moiré patterns obtained from the crystals.

**12468.** Negas, T., Roth, R. S., **Phase equilibria and structural relations in the system  $\text{BaMnO}_{3-x}$** , *J. Solid State Chem.* **3**, 323-339 (1971).

Key words: Barium-manganese oxides; crystal structures; oxidation-reduction; phase equilibria; system  $\text{BaMnO}_3$ .

The system  $\text{BaMnO}_{3-x}$  ( $0 \leq x < 0.5$ ) in air was investigated by gravimetric, quenching, single-crystal and powder-x-ray diffrac-



tion studies. Below 1150 °C hexagonal, two-layer BaMnO<sub>3</sub> ( $a = 5.699 \text{ \AA}$ ,  $c = 4.817 \text{ \AA}$ ) is stable. Above 1150 °C a series of anion deficient BaMnO<sub>3-x</sub> phases exists. With increasing temperature, these include a rhombohedral 15-layer form ( $a = 5.681 \text{ \AA}$ ,  $c = 35.377 \text{ \AA}$ ; hexagonal indexing) and hexagonal 8-layer ( $a = 5.699 \text{ \AA}$ ,  $c = 18.767 \text{ \AA}$ ), 6-layer ( $a = 5.683 \text{ \AA}$ ,  $c = 14.096 \text{ \AA}$ ), 10-layer ( $a = 5.680 \text{ \AA}$ ,  $c = 23.373 \text{ \AA}$ ) and 4-layer ( $a = 5.672 \text{ \AA}$ ,  $c = 9.319 \text{ \AA}$ ) forms. The 6-layer modification is not of the hexagonal BaTiO<sub>3</sub>-type. A simple orderly structural sequence involving a progressive increase of cubic-type layer stacking with increasing temperature characterizes the phases prepared. Influence of anion stoichiometry on phase formation is considered.

**12469.** Newman, M., Units in cyclotomic number fields, *J. Reine Angew. Math.* **250**, 1-11 (1971).

Key words: Cyclotomic units; diophantine equations; roots of unity.

Conditions for a unit in a cyclotomic number field to be a power of another unit in that field are derived, and the results applied to show that equations such as  $1 + \zeta = \alpha^r$ ,  $\zeta$  a primitive  $n$ th root of unity,  $n$  odd and  $> 3$ , have only the trivial solution  $r = 1$ ,  $\alpha = 1 + \zeta$ .

**12470.** Plitt, K. F., Utech, H. P., Flammability of turnout coats tested, *Fire Eng.* **124**, No. 10, 60 (Nov. 1971).

Key words: Bunker coats; fabric flammability; firefighter clothing; fireman; flame resistance; turnout coats.

Flame resistance tests (Vertical Burn Method) were conducted on four commercially purchased firefighters' turnout coats. Each coat had three fabric layers: outer shell, interlining, and inner lining. The results show that 2 of 3 fabric layers in each coat produced a char length of 12 inches.

**12471.** Powell, F. J., Research needs in thermal insulation, (Proc. Symp. Thermal Insulation, Columbus, Ohio, Feb. 5-8, 1968), ASHRAE (Amer. Soc. Heat. Refrig. Air-Cond. Eng.) *Bull. Thermal Insulation*, pp. 14-17 (1971).

Key words: Performance coefficients; thermal insulation; transient heat transfer.

The role that research in respect to thermal insulation can play will be examined in this paper. Efforts to develop better insulation materials through research and to search for better methods of application need to be continued, and, in addition, the need to develop methods of measurement, performance coefficients, load calculations and applications based on transient or dynamic conditions of heat flow rather than steady-state concepts will be discussed. With the advent of computers, the sophistication required for treating the complex transient heat flow problems becomes feasible and the time has arrived for research to enable accurate estimation of transient loads that are indicative of actual performance.

**12472.** Rasberry, S. D., Applications of x-ray analysis, 20th Annual Denver X-Ray Conference, Denver, Aug. 11-13, 1971, *Appl. Opt.* **10**, No. 12, 2795 (Dec. 1971).

Key words: Applied x-ray analysis; conference report; material analysis; x-ray diffraction; x-ray fluorescence.

In this meeting report of the 20th Annual Denver X-ray Conference, the general nature of this series of meetings is outlined. Some details specific to the papers presented this year are reported.

**12473.** Rosenstock, H. M., Harmonic oscillator Franck-Condon factors for the ionization of N<sub>2</sub>O, *Intern. J. Mass Spectrom. Ion Phys.* **7**, 33-39 (1971).

Key words: Franck-Condon factor; ionization; N<sub>2</sub>O; N<sub>2</sub>O<sup>+</sup>; photoelectron spectroscopy.

Harmonic oscillator Franck-Condon factors have been calculated for the ionization of N<sub>2</sub>O. The Franck-Condon factors are quite sensitive to the form of the valence force field for the ion. The results are in fair agreement with experimental values obtained by photoelectron spectroscopy.

**12474.** Rubin, S., Oettinger, F. F., Thermal hysteresis and its possible effect in restricting the hot-spot-free operating range of some power transistors, *IEEE Trans. Electron Devices* **ED-18**, No. 6, 393-394 (June 1971).

Key words: Current constriction; DC current gain; hot-spot screening; methods of measurement; power transistors; reliability; thermal hysteresis; thermal resistance; thermographic measurements; transistor screening.

Studies conducted on a number of silicon power transistors indicate that for some devices a hot spot, once formed, will remain even though the power dissipation is reduced to a level at which operation was previously free of hot spots. The hot spot can be eliminated only by a significant reduction in power dissipation from the level at which the hot spot first appeared. The effect of the hot spot on reliable device operation is discussed.

**12475.** Saylor, C. P., Refractive index, Chapter in *The Characterization of Chemical Purity of Organic Compounds*, L. A. K. Staveley, ed., pp. 67-79 (July 1971).

Key words: Contamination; differential refractometer; identification; impurity; interferometer; purity; refractive index; refractometer.

Refractive index is not particularly valuable in the measurement of purity because the effects of impurities upon the property are indeterminate. A given impurity may raise, lower, or leave the refractive index unchanged. Those impurities that will most probably be present are, ordinarily, least certain to affect the refractive index. Still, a sample that has exactly the same refractive index as the perfectly pure material can usually be presumed to have high purity, since contaminants are unlikely to compensate precisely, and the more accurately the property is measured the more valid is the presumption. The methods of determination using liquid samples and the limits of accuracy to which the measurements of refractive index can be pressed will be discussed.

The situation with solids is different. In most cases, an impurity influences the refractive index of a solid very little if at all. Refractive index differences can be used to recognize isolated pockets of impurity, however, and by estimation and summation of the volumes of such outcroppings useful clues to the degree of contamination on that are not otherwise available can be secured.

**12476.** Schade, P. A., Signal decoder eliminates jitter, *Electron. Design* **19**, No. 24, 1 (Nov. 25, 1971).

Key words: False counts; incremental encoder; jitter; up-down counter; 90° phase decoder.

The two main types of decoders used with incremental shaft encoders are discussed. Emphasis is given to the problem of decoding signals which result from an oscillating shaft. A particular decoder circuit designed and tested by the author is presented.

**12477.** Schwartz, R. B., Heaton, H. T., II., Schrack, R. A., High-accuracy total-cross-section measurements with the NBS Linac, (Proc. Symp. Neutron Standards and Flux Normalization, Argonne National Laboratory, Argonne, Ill., Oct. 21-23, 1970), *AEC Symp. Series Neutron Standards and Flux Normalization* **23**, 377-384 (Aug. 1971).

Key words: Cross section; MeV; neutron; time-of-flight.

A high-accuracy fast-neutron time-of-flight spectrometer used for neutron energies between 0.5 and 20 MeV is described. The neutrons are produced by a 2-nsec-wide electron-beam pulse from the National Bureau of Standards Linac. The resolution, with a 40-m flight path, is approximately 0.1 nsec/m, and the accuracy of the measurements is estimated to be 1%.

**12478.** Schwartz, R. B., Schrack, R. A., Heaton, H. T., II., A search for structure in the *N-P* total cross section, (Proc. Neutron Standards and Flux Normalization Symp., Argonne National Laboratory, Argonne, Ill., Oct. 21-23, 1970. Sponsored by the European American Nuclear Data Committee), *AEC Symposium Series* **23**, pp. 57-62 (Aug. 1971).

Key words: Cross section; hydrogen; neutron; *n-p*; scattering; time-of-flight.

High-precision measurements of the *n-p* total cross section below 30 MeV show no evidence of any structure. A careful measurement of the differential scattering cross section also shows no evidence of any anisotropy.

**12479.** Swartzendruber, L. J., Bennett, L. H., Use of ultrasonics in laboratory development tests of cupro-nickel alloys for desalination, *Desalination* **9**, 387-389 (June 1971).

Key words: Alloys; corrosion; cupro-nickel; high velocity; sea-water; ultrasonics.

Ultrasonic agitation of the salt-water bath is suggested as a simple laboratory corrosion test method for evaluating the relative performance of alloys intended for use at moderate or high-sea water velocities.

**12480.** Allan, D. W., Gray, J. E., Comments on the October 1970 *Metrologia* paper "the U.S. Naval Observatory clock time reference and the performance of a sample of atomic clocks," *Metrologia* **7**, No. 2, 79-82 (Apr. 1971).

Key words: Atomic clock; clock weighting factors; flicker noise; frequency stability; noise; synchronization; time; time scale; time scale precision.

The paper cited in the title by Winkler, Hall, and Percival (WHP) documents some important aspects of the widely referenced United States Naval Observatory (USNO) Time Scale system. We augment the text of WHP regarding the mutual synchronization to within 5  $\mu$ s of the Time Scale, UTC(USNO), with another widely referenced time scale, the National Bureau of Standard UTC(NBS) Time Scale. We show that some of the information available to WHP can be utilized to give even more precision to the USNO Time Scale system and that some of that information has been improperly interpreted causing some errors by WHP in their conclusions regarding time scale precision, clock weighting factors, and drift in rate of the time scale.

**12481.** Andrews, J. R., Horizontal time base sweep generator for a traveling wave oscilloscope, *IEEE Trans. Nucl. Sci.* **NS-18**, No. 5, 3-8 (Oct. 1971).

Key words: High voltage pulse; nanosecond; oscilloscope; pulse generator; sweep generator; time base; traveling wave oscilloscope.

This paper describes the design, construction, and performance of a time base generator for use with a cathode ray tube capable of displaying fractional nanosecond transients. The generator was designed for use with a traveling wave cathode ray tube having a simple electrostatic time base deflection structure. When operating into the deflection plates (total capacitive load of 25 pF), the generator produced a total ramp excursion of  $-4$  kV with a maximum average slope of about  $-450$  V/ns. with a

maximum repetition rate of 10 kHz. The ramp slope may be decreased continuously by a control voltage. The generator may also be operated into a 50 ohm load for the production of a  $-750$  V transition with 10%-90% transition time of 4.8 ns.

**12482.** Bates, R. G., Paabo, M., Measurement of pH, *Handbook of Biochemistry*, H. A. Sober, ed., 2d Edition, pp. J227-J233 (Chemical Rubber Company, Cleveland, Ohio, Jan. 1971).

Key words: Acidity; glass electrode; indicators; pH; standardization.

The operational definition of pH, in the form endorsed by the International Union of Pure and Applied Chemistry, is presented. The preparation of standard reference solutions for pH measurements is described and the choice of electrodes and measurement techniques is discussed. The proper interpretation of pH numbers is set forth briefly, and procedures for pH measurement with indicators are described.

The revised version includes the addition of two new primary pH standards to tables 1 and 3, coefficients for calculating the temperature dependence of pH in table 2, and a collection of pH values for miscellaneous buffer solutions.

**12483.** Berry, R. J., Riddle, J. L., Intercomparison of oxygen boiling point realizations in standards laboratories, *Metrologia* **7**, No. 2, 56-58 (1971).

Key words: IPTS-68; oxygen point.

The experimental realizations of the normal boiling point of oxygen maintained in several national standards laboratories are compared.

**12484.** Block, S., The user's viewpoint on x-ray diffraction safety standards, *Proc. Conf. Radiation Safety in X-Ray Diffraction and Spectroscopy*, University of Pennsylvania, Philadelphia, Pa., Jan. 6-7, 1970, pp. 211-221 (Sept. 1971).

Key words: Diffraction; fluorescence analysis; radiation safety; x rays.

The user's point of view on safety standards for x-ray diffraction and fluorescence analysis equipment is presented as part of a panel discussion.

**12485.** Brady, G. W., Gravatt, C. C., Jr., Determination of the radial distribution function and the direct correlation function of spheres by x-ray small-angle scattering, *J. Chem. Phys.* **55**, No. 10, 5095-5101 (Nov. 15, 1971).

Key words: Hard sphere fluid; liquids; radial distribution function; small-angle x-ray scattering.

An experimental determination of the pair and direct correlation functions of polystyrene latex spheres in the high-density limit has been made. From these the pair potential for hard spheres has been calculated. The significance of the functions as they bear on the Percus-Vevick and the hypernetted chain approximation is discussed.

**12486.** Braun, W., Carlone, C., Carrington, T., Van Volkenburgh, G., Young, R. A., Collisional deactivation of  $H(2^2P)$  fluorescence, *J. Chem. Phys.* **53**, No. 11, 4244-4248 (Dec. 1, 1970).

Key words: Deactivation; fluorescence; hydrogen atoms; quenching.

Collision cross sections for deactivation of  $H^*(n=2)$  at 300 K have been measured by observations of the quenching of Lyman- $\alpha$  fluorescence in a discharge flow system. The quenchers (with cross section in  $\text{\AA}^2$ ) are  $H_2(84 \pm 8)$ ,  $D_2(84 \pm 8)$ ,  $N_2(62 \pm 6)$ ,  $He(< 3)$ . For  $H^* + H_2$ , less than 1% of the total quenching produces



ions. Care has been taken to work with systems optically thin in Lyman  $\alpha$  so that the rate of escape of radiation, which is the reference to which the quenching rate is compared, is not reduced by resonance trapping.

**12487.** Carter, G. C., Swartz, J. C., **Nuclear magnetic resonance Knight shifts and quadrupole effects in transition metal diborides**, *J. Phys. Chem. Solids* **32**, 2415-2421 (Jan. 1971).

Key words: Electric quadrupole coupling constant; Knight shift; NMR;  $\text{ScB}_2$ ; transition metal diborides.

Nuclear magnetic resonance data for  $\text{ScB}_2$ ,  $\text{YB}_2$  and  $\text{MnB}_2$  are presented. These data together with earlier NMR data provide a complete picture of the  $3d$  and  $4d$  transition metal diborides:  $\text{ScB}_2$  through  $\text{MnB}_2$  and  $\text{YB}_2$  through  $\text{MoB}_2$ . The Knight shifts, electric quadrupole coupling constants, and linewidths of the central resonance of the  $^{45}\text{Sc}$  and  $^{11}\text{B}$  nuclei in  $\text{ScB}_2$  are essentially temperature independent in the range 4–300 K. The boron Knight shifts  $\mathcal{K}(\text{B})$  are 0.00(1)%,  $-0.004(10)\%$  and  $-0.05(2)\%$  in  $\text{ScB}_2$ ,  $\text{YB}_2$  and  $\text{MnB}_2$ , respectively.  $\mathcal{K}(\text{Sc}) = 0.07(1)\%$  and  $\mathcal{K}(\text{Y}) = 0.20(3)\%$  in the respective diborides. The difference between these values and the higher values for metallic Sc and Y is attributed primarily to reduced orbital and Pauli contributions. For the  $3d$  series  $\text{ScB}_2$  to  $\text{MnB}_2$ , the Knight shifts, electronic specific heats, magnetic susceptibilities and transport properties indicate increasing  $d$ -electron character with increasing group number. The quadrupole coupling constant of  $^{11}\text{B}$  across both  $3d$  and  $4d$  series does not correlate with the  $c/a$  ratio or unit cell volume. This may indicate deviation of the boron atoms from a planar configuration.

**12488.** Cezairliyan, A., **Recent developments in thermophysical properties research**, *Proc. Committee Thermophysical Properties, Washington, D.C., Dec. 1, 1971, HTD-3*, 12-13 (American Society of Mechanical Engineers, New York, N.Y., 1971).

Key words: High-speed measurements; high temperature; thermodynamics; thermophysical properties.

Recent developments in high-speed measurement of thermophysical properties at high temperatures are summarized. Emphasis is placed on methods that allow the performance of measurements in subsecond duration on electrically conducting substances in the solid phase. High-speed measurements of properties, such as specific heat, electrical resistivity, hemispherical total emittance, normal spectral emittance, and temperatures and energies of phase transitions and transformations are described.

**12489.** Cooper, M. J., **Various expansions in thermodynamic scaling**, *Phys. Rev. A* **5**, No. 1, 318-320 (Jan. 1972).

Key words: Critical region; equation of state; scaling laws; thermodynamic scaling.

Several recently proposed general extensions of thermodynamic scaling are compared and a single comprehensive form suggested.

**12490.** Dean, J. A., Rains, T. C., **Standard solutions for flame spectrometry**, Chapter 13 in *Flame Emission and Atomic Absorption Spectrometry II*, 327-339 (Marcel Dekker, Inc., New York, N.Y., July 1971).

Key words: Atomic absorption spectrometry; flame emission spectrometry; standard solutions; stock solutions.

The availability of standard samples and high-purity materials for preparing reference and standard solutions is an important criterion for the solution of an analytical method. For application in the fields of atomic absorption and flame emission spectrometry various types, as well as the source, of standard samples and high purity materials are listed. Procedures for prepar-

ing standard stock solutions for 74 elements and special solutions for a variety of matrices are described.

**12491.** De Simone, D. V., **Moving to metric makes dollars and sense**, *Harvard Bus. Rev.*, pp. 100-111 (Jan.-Feb. 1972).

Key words: Business and industry; economy; education; international relations; international standards; international trade; metric; technology assessment.

The article will be a summary of the report, "A Metric America," which evaluates and distills the findings of the U.S. Metric Study in which thousands of individuals, firms and organized groups, representative of our society, participated. On the basis of all the evidence marshalled in the Study, the report concludes that the United States should change to the metric system through a coordinated national program.

**12492.** Dise, J. R., **Recent developments in cement testing**, *Proc. General Technical Committee, Portland Cement Association, San Francisco, Calif., Sept. 22, 1971, Mill Session Papers M-197*, 34-42 (1971).

Key words: Hydraulic cement; testing of cement.

This review of recent developments in cement testing has been prepared for the purpose of recording some of the unpublished information about the testing of hydraulic cements that has come to the attention of the author through his work with Committee C-1 on Cement of the American Society for Testing and Materials, and the Cement and Concrete Reference Laboratory at the National Bureau of Standards.

**12493.** Escalante, E., Kruger, J., **Stress corrosion cracking of pure copper**, *J. Electrochem. Soc.* **118**, No. 7, 1062-1066 (July 1971).

Key words: Copper; cupric acetate; kinetics; oxidation; stress corrosion; tarnish film.

It is known that the rate of tarnish film formation is an important factor in the stress corrosion cracking (SCC) of brass. Because copper immersed in cupric acetate and sulfate solutions has tarnish film growth rates comparable to those found for brasses susceptible to SCC, it should undergo cracking in such solutions if kinetics play a role. It was found that pure copper is susceptible to cracking in cupric acetate solution but not in cupric sulfate. Light, which retards film formation on copper, but not corrosion, prevents stress cracking in the cupric acetate solution. In the absence of stress, oxide forms all over the copper surface, while stress concentrates oxide formation at the grain boundaries. These experiments point to a brittle-film rupture mechanism of stress cracking.

**12494.** Fraker, A. C., Ruff, A. W., Jr., **Studies of oxide film formation on titanium alloys in saline water**, *Corrosion Sci.* **11**, 763-765 (Dec. 1971).

Key words: Electron microscopy; hot saline water corrosion; oxide films; titanium; titanium alloy corrosion.

Oxide films formed on five titanium alloys were characterized after corrosion in 3.5wt.% NaCl solutions over the temperature range of 100-200 °C. Electron transmission microscopy and electron diffraction of corroded thin foils showed the oxide film to be  $\text{TiO}$  and  $\text{Ti}_2\text{O}_3$  in the early corrosion stages and to change in the 150-200 °C temperature range to a final surface oxide,  $\text{TiO}_2$  (anatase).

**12495.** Goldstein, J. I., Yakowitz, H., **Metallic inclusions and metal particles in the Apollo 12 lunar soil**, Chapter in *Proceedings 2d Lunar Science Conference, Houston, Texas, Jan. 1971*, 1, 177-191 (MIT Press, Cambridge, Mass., Mar. 1971).

**Key words:** Electron probe microanalyzer; lunar age; lunar materials; meteorites; scanning electron microscopy.

Almost all the reduced metal in the Apollo 12 lunar soil was found as inclusions in the individual soil particles. The inclusions contain  $< 0.1 - > 20.0$  weight% Ni and  $< 0.1 - 2.5$  weight% Co. These Ni and Co contents are similar to those measured for metal grains in Apollo 12 igneous rocks. Curves of Ni vs. Co contents for meteoritic metal were used to differentiate the meteoritic metal component from the lunar component. On this basis over 80% of the metal areas examined had Ni and Co contents outside of the known meteoritic composition range and were derived from the lunar igneous rocks. The presence of the meteoritic inclusions in the soil particles can be explained by low velocity impacts in the lunar soil during major meteoritic bombardment on the moon.

Six individual metal particles  $> 125 \mu\text{m}$  in size, separated from 50 grams of Apollo 12 soil, were studied. Four of the six particles are meteoritic. Two of the meteoritic particles exhibit deformation bands produced by peak shock pressures  $< 150$  kb. The other two meteoritic particles  $\sim 1/2$  mm in diameter were remelted during impact on the moon. Dendrites of Fe-Ni are visible in one and a phosphide-kamacite eutectic structure is present in the other. The structures and compositions of the phases present in these particles indicate either slow cooling or a reheating of these particles on the moon's surface in the 500-600 °C temperature range for a year or more. Most of the meteoritic particles studied were probably originally pieces of chondrites.

**12496.** Hastie, J. W., Plante, E. R., *Entropy in isotopic systems, High Temp. Sci.* 3, No. 5, 412-414 (Sept. 1971).

**Key words:** Entropy; isotopes; symmetry number; third law.

Many current textbooks and even the research literature appear inadequate in recognizing or discussing certain entropy conventions. The present article elaborates on this question with particular reference to a recent research article that amply demonstrates the errors that can result from the misunderstanding of entropy conventions in isotopic systems.

**12497.** Heydemann, P., *Ultrasonic measurements at very high pressures, Phys. Acoust.* 8, 203-236 (1971).

**Key words:** Equation of state; high pressure; liquids; solids; ultrasonic measurements.

Ultrasonic measurements are used to determine equations of state for solids and liquids at very high pressures. These measurements are made in piston and cylinder, piston and die, belt or girdle and anvil apparatus. A particularly useful apparatus is the piston and die system with fluid container which is described in greater detail. Often ultrasonic measurements can be combined with isothermal compression measurements to give additional information on  $c_p/c_v$ ,  $\gamma_G$  and  $\alpha$ . Examples of results and estimates of the attainable accuracy are given.

**12498.** Hockey, B. J., *Plastic deformation of aluminum oxide by indentation and abrasion, J. Am. Ceram. Soc.* 54, No. 5, 223-231 (May 1971).

**Key words:** Abrasion; alumina; annealing; dislocations; electron microscopy; indentation; plastic deformation; surface regions; transmission electron microscopy; twinning.

Transmission electron microscopy provided direct evidence that plastic deformation occurs during the room-temperature indentation and abrasion of  $\text{Al}_2\text{O}_3$ . Examination of single-crystal and polycrystalline specimens showed that high densities of dislocations are produced within the near-surface regions by mechanical polishing with a fine diamond compound ( $0.25 \mu\text{m}$ )

and that plastic deformation by both slip and mechanical twinning occurs during the placement of Vickers microhardness indentations. The occurrence of plastic deformation in this normally brittle material is considered to be a consequence of the nature and magnitude of the local stresses developed under pointed indenters and irregularly shaped abrasive particles. Preliminary results on the effect of annealing on the retained substructure are also presented. Annealing at 900 °C and higher resulted in the reduction of residual stresses through the motion of dislocations and their rearrangement into lower-energy configurations.

**12499.** Huie, R. E., Herron, J. T., Davis, D. D., *Absolute rate constants for the reaction of atomic oxygen with 1-butene over the temperature range of 259-493 K, J. Phys. Chem.* 75, No. 25, 3902-3903 (1971).

**Key words:** Atomic oxygen; flash photolysis; kinetics; 1-butene.

Rate constants for the reaction of atomic oxygen with 1-butene have been measured over a temperature range of 259 to 493 K using the flash photolysis-resonance fluorescence technique. No dependence of rate constants on pressure or reactant concentration was observed.

The rate constant for the reaction of atomic oxygen with 1-butene was found to be:

$$k = 1.46 \pm 0.15 \times 10^{-11} \exp \left( \frac{-760 \pm 60 \text{ cal mol}^{-1}}{RT} \right) \text{ cm}^3 \text{ molecule sec}^{-1}.$$

**12500.** Johns, J. W. C., Olson, W. B., *The infrared spectrum of thioformaldehyde, J. Mol. Spectry.* 39, No. 3, 479-505 (Sept. 1971).

**Key words:** High resolution; infrared; rotational constants; short lived molecule; spectrum; thioformaldehyde.

The infrared spectrum of thioformaldehyde ( $\text{H}_2\text{CS}$ ) has been observed in the C-H stretching region. The spectrum was obtained under conditions of high resolution and rotational analyses have been carried out on the three observed bands. The main results (in  $\text{cm}^{-1}$ ) for the excited states are:

Band	$\nu_0$	A	B	C
$\nu_3$	3024.61	9.675	0.5893	0.5554
$\nu_1$	2971.03	9.648	0.5907	0.5542
$2\nu_6(?)$	2877.11	9.821	0.5936	0.5533

Several local perturbations have been observed in the two fundamentals  $\nu_3$  and  $\nu_1$ . These are presumably caused by overtones and combinations of the lower lying fundamentals but it has not been possible to make specific assignments of the perturbing levels.

**12501.** Johnson, D. R., Lovas, F., *A new look at the laboratory microwave spectrum of cyanoacetylene, Astrophys. J.* 169, 617-619 (Nov. 1, 1971).

**Key words:** Cyanoacetylene; hyperfine structure; interstellar microwave emission; laboratory microwave spectrum; radio astronomy; rotational transitions.

Laboratory measurements have been made on several transitions in cyanoacetylene with potential application to radio astronomy. Observations of  $J=1 \leftarrow 0$  and  $J=2 \leftarrow 1$  rotational transitions are reported for the isotopic species  $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ ,  $\text{H}^{13}\text{C}^{12}\text{C}^{12}\text{C}^{14}\text{N}$ , and  $\text{H}^{12}\text{C}^{12}\text{C}^{12}\text{C}^{15}\text{N}$ . Measurement errors and resolution of hyperfine structure are discussed in some detail.

**12502.** Julienne, P. S., Krauss, M., Wahl, A. C., *Hartree-Fock energy curves for  $X^2\Pi$  and  $2\Sigma^+$  states of  $\text{HF}^+$ , Chem. Phys. Letters* 11, No. 1, 16-20 (Sept. 15, 1971).



Key words:  $D_0^0(\text{HF})$ ;  $D_e(\text{HF}^+)$ ; dissociation energy; Hartree-Fock; photoelectron spectra; vibrational energy levels.

Hartree-Fock energy curves have been calculated for the  $X^2\Pi$  and  $^2\Sigma^+$  states of  $\text{HF}^+$  and applied to an analysis of the photoelectron spectra of HF. The  $^2\Sigma^+$  energy curve is found to have a barrier about 0.07 eV high due primarily to a repulsive ion-quadrupole interaction, and a depth of 0.37 eV. This curve will support two bound states and one shape resonance with a half-width of 0.015 eV. The energy curves are probably accurate to 0.1 eV but the analysis shows that results accurate to within 0.03 eV are required to resolve the experimental questions on the dissociation energy for the ground state of HF. The most recent experimental photoelectron results of Berkowitz (following article) encouraged a model calculation of the vibrational states of the  $^2\Sigma^+$  state. Assuming a dissociation energy of 0.45 eV and retaining the barrier three bound and one shape resonance vibrational levels are calculated for  $\text{HF}^+$  in agreement with the results reported by Berkowitz.

**12503.** Kirby, R. K., Rothrock, B. D., **Thermal expansion of platinum to 1900 K and reference materials for thermophysical properties**, *Proc. European Conf. Thermophysical Properties of Solid Materials at High Temperatures, Baden-Baden, Germany, Nov. 11-13, 1968*, pp. 600-620 (Feb. 1970).

Key words: Platinum; standard reference materials; thermal expansion.

The thermal expansion of two specimens of platinum has been measured with a precision optical comparator. A controlled-gradient vacuum furnace was used to heat each specimen to temperatures between 1000 and 1900 K. Within this temperature range the linear thermal expansion of the two specimens is given by

$$\frac{L_t - L_{293}}{L_{293}} \times 10^6 = -2685 + 8.972 T + 2.505 \times 10^{-4} T^2 + 4.641 \times 10^{-7} T^3.$$

The National Bureau of Standards is actively engaged in certifying several standard reference materials for thermophysical properties. These include expansivity standards of vitreous silica, borosilicate glass, single-crystal sapphire, copper and tungsten and a calorimetric standard of single-crystal sapphire.

**12504.** McAlister, A. J., Williams, M. L., Cuthill, J. R., Dobbyn, R. C., **Relation between the 5d band structure and soft x-ray  $N_{6,7}$  emission spectrum of Au**, *Solid State Commun.* **9**, 1775-1777 (July 1971).

Key words: Band structure; emission spectrum; gold;  $N$  spectrum; soft x rays.

The  $N_{6,7}$  soft x-ray emission spectrum of Au (5d to 4f transition) has been measured. Distinct structural features are observed. The absolute positions in photon energy of these features are derivable from x-ray and u.v. induced photo-emission spectra. In turn, these experiments agree well with recent band calculations for Au and thus offer further support of the utility of the single particle description of the occupied band structure of metals.

**12505.** Mentall, J. E., Gentieu, E. P., Krauss, M., Neumann, D., **Photoionization and absorption spectrum of formaldehyde in the vacuum ultraviolet**, *J. Chem. Phys.* **55**, No. 12, 5471-5479 (Dec. 15, 1971).

Key words: Formaldehyde; integrated oscillator strength; photoionization coefficient; Rydberg spectrum; SCF calculations; vacuum UV spectrum.

Absorption and photoionization coefficients have been measured for  $\text{H}_2\text{CO}$  in the 600-2000-Å region. Integrated oscillator

strengths were determined for a number of strong Rydberg transitions above 1200 Å. From the photoionization curve the first adiabatic ionization potential was found to be  $10.87 \pm 0.01$  eV. As an aid in interpreting the absorption spectrum, theoretical calculations were made using a single-configuration self-consistent field procedure for the Rydberg states and a model which included mixing between the Rydberg and valence states. On this basis, weak absorption features between 1340 and 1430 Å have been assigned to the  $^1B_1(\sigma \rightarrow \pi^*)$  valence state. The  $^1A_1(\pi \rightarrow \pi^*)$  valence state is deduced to be strongly autoionized just above the  $^2B_2$  ionization limit.

**12506.** Mielczarek, S. R., Miller, K. J., **Dependence of generalized oscillator strengths of  $\text{H}_2\text{O}$  on momentum transfer**, *Chem. Phys. Letters* **10**, No. 4, 369-370 (Aug. 15, 1971).

Key words: Electronic excitation; generalized oscillator strength;  $\text{H}_2\text{O}$ ; inelastic electron scattering; momentum transfer.

Experimental results on the dependence of generalized oscillator strengths of water on momentum transfer, showing the appearance of extrema and characteristic features in the electron scattering spectra are reported and discussed.

**12507.** Okabe, H., **Fluorescence predissociation of sulfur dioxide**, *J. Amer. Chem. Soc.* **93**, No. 25, 7095-7096 (1971).

Key words: Fluorescence; predissociation; quenching;  $\text{SO}_2$ .

The fluorescence intensity of  $\text{SO}_2$  was measured as a function of incident wavelength in the region 2000 to 2300 Å where dissociation is expected to compete with fluorescence.

A sudden decrease of the fluorescence intensity was observed below the incident wavelength 2189 Å, corresponding to the photon energy of 5.66 eV which agrees almost exactly with the thermochemical threshold of 5.65 eV for dissociation. This indicates that the photodissociation starts to compete with the fluorescence above this photon energy. The quenching rate by Ar of the excited  $\text{SO}_2$  produced at 2208 Å is  $5 \times 10^{-11} \text{ cm}^3 \text{ molecules}^{-1} \text{ sec}^{-1}$  on the basis of the lifetime of 9 ns calculated from the integrated absorption coefficient. The lifetime decreases to 3.2 ns for the excited state at 2189 Å because of the predissociation.

**12508.** Reneker, D. H., Colson, J. P., **Annealing and melting of polyoxymethylene crystals polymerized within irradiated trioxane crystals**, *J. Appl. Phys.* **42**, No. 12, 4606-4614 (Nov. 1971).

Key words: Annealing of polyoxymethylene; polyoxymethylene; polyoxymethylene crystals; solid state polymerization; trioxane.

Morphological changes produced by the annealing and melting of the polyoxymethylene crystals that polymerize inside irradiated trioxane crystals were observed. The crystals in which the polyoxymethylene chains were oriented parallel to the threefold axis of the trioxane underwent major reorganization when held at 184 °C for 30 sec. The polyoxymethylene crystals in which the chain axis was inclined at a large angle with respect to the threefold axis of the trioxane transformed and melted at temperatures approximately 5 °C lower.

**12509.** Robertson, B., **Wyler's expression for the fine-structure constant  $\alpha$** , *Phys. Rev. Letters* **27**, No. 22, 1545-1547 (Nov. 29, 1971).

Key words: Conformal group; fine structure constant; relativistic quantum theory; symmetric spaces.

Wyler's expression for  $\alpha$  in terms of the Euclidean volumes of certain bounded spaces agrees with experiment only if the radius of these spaces is arbitrarily chosen to equal 1. However, the

relationship between these spaces and the invariance group  $O(n,2)$  of the  $n$ -dimensional wave equation is independent of the radius. There is no known reason for setting the radius equal to one.

- 12510.** Romberg, E. F., Wall, N. S., Blum, D., Lightbody, J. W., Jr., Penner, S., **Elastic scattering of 60-120 MeV electrons from  $^{46,48,50}\text{Ti}$** , *Nucl. Phys. A* **173**, 124-128 (1971).

**Key words:** Elastic electron scattering; nuclear charge distribution; nuclear radii; titanium isotopes.

The elastic electron scattering from the isotopes of  $^{46,48,50}\text{Ti}$  has been measured at an angle of  $127.5^\circ$ . The ratios of the cross sections were analysed with a partial-wave analysis for a Fermi-shaped charge distribution and the parameter variations were deduced. Some consequences of these results are discussed.

- 12511.** Schooley, J. F., Soulen, R. J., Jr., **Superconductive transitions suitable as thermometric fixed points**, E. Kanda, ed., *Proc. XII Conf. Low Temperature Physics, Kyoto, Japan, Sept. 3-10, 1970*, pp. 833-834 (Keigaku Publishing Co., Tokyo, Japan, Mar. 1971).

**Key words:** Elements; fixed points; reproducibility; superconductors; thermometry; transition widths; wire samples.

We have shown that annealed wire samples of Pb, In, Al, Ga, and Zn, when simply prepared and mounted, exhibit superconductive transitions using A.C. susceptibility techniques which are sharper than one millikelvin. These transitions are reproducible to a millikelvin after many thermal cycles over a twenty-month period, suggesting their use as thermometric fixed points.

- 12512.** Velapoldi, R. A., Menis, O., **Formation and stabilities of free bilirubin and bilirubin complexes with transition and rare-earth elements**, *Clin. Chem.* **17**, 1165-1170 (1971).

**Key words:** Bilirubin; bilirubin-lanthanide complexes; bilirubin-transition metal complexes; biliverdin; solvents; stability; tetrapyrroles.

We investigated complexes formed between bilirubin and transition or rare-earth elements, and their relative stabilities. Relative rates of complex formation were analogous to metal-porphyrin and metal complex stabilities, according to the Irving-Williams series. Transition metals that formed strong, square planar complexes caused rapid bilirubin degradation. Iron(II) was oxidized to iron(III) in the bilirubin complex. Of the lanthanide complexes, only samarium(III) showed covalent bonding tendencies. Comparative molar absorptivities were calculated for several of the metal-bilirubin complexes. The stability of bilirubin in several solvents and under various experimental conditions is reported. At room temperature, bilirubin photooxidizes to biliverdin on exposure to laboratory light.

- 12513.** Wagner, H. L., **Standard reference materials for polymer characterization at the National Bureau of Standards**, *Polymer Preprints, ACS* **12**, No. 2, 770-774 (1971).

**Key words:** Characterization; gel permeation chromatography; light scattering; molecular weight; molecular weight distribution; osmometry; SRM 705; SRM 706; SRM 1475; SRM 1476.

The National Bureau of Standards now has available a total of four Polymer Standard Reference Materials, designed for use in the calibration of instruments employed in polymer characterization. Polystyrene is available in narrow (SRM 705) and broad (SRM 706) molecular weight distributions, while polyethylene whole polymers are available in both high density linear (SRM 1475) and low density branched (SRM 1476) materials. After careful measurements of sample homogeneity,

these materials were characterized with respect to weight and number average molecular weight, limiting viscosity number in several solvents, and for the polyethylenes, A.S.T.M. density and A.S.T.M. flow rate. The molecular weight of the branched material has not been certified. In addition, the molecular weight distribution of the linear polyethylene was carefully determined; consequently it is well suited for calibration of gel permeation chromatographs at high temperatures in the molecular weight range of  $10^3$  to  $10^6$ .

- 12514.** Waynant, R. W., Ali, A. W., Julienne, P. S., **Experimental observations and calculated band strength for the  $\text{D}_2$  Lyman band laser**, *J. Appl. Phys.* **42**, No. 9, 3406-3408 (Aug. 1971).

**Key words:** Adiabatic approximation; band strengths;  $\text{D}_2$  Lyman emission; emission wavelengths; traveling wave excitation; vacuum ultraviolet laser.

Experimental observations have been made of vacuum ultraviolet laser emission in the Lyman band of  $\text{D}_2$ . Fourteen lines from 1568 to 1614 Å have been measured to have a total peak power of nearly 1 MW in a short ( $\sim 1$  nsec) pulse. To facilitate identification of the laser wavelengths, optical functions were calculated using the adiabatic correction to the usual Born-Oppenheimer approximation. The theory predicts the most probable transitions and these wavelengths agree with experiment to within 0.1-0.2 Å.

- 12515.** Wells, T. E., Gard, E. F., **An integrated system for the precise calibration of four-terminal standard resistors**, (Proc. Conf. Electronic and Electrical Measurements and Test Instrument Conference, Ottawa, Canada, June 1-3, 1971), *IEEE Trans. Inst. Meas.* **IM-20**, No. 4, 253-257 (Nov. 1971).

**Key words:** Ampere-turn balance; flux balance; standard resistor; voltage balance.

A description is given of the system currently in use at the National Bureau of Standards for measurements of  $1 - \Omega$  standard resistors of the Thomas type. A tenfold improvement in accuracy over the former method has been realized. Resistors of this type are now reported to eight decimal places with a total uncertainty of 0.08 ppm. The latter figure includes a three-standard-deviation limit for random errors plus an estimate of systematic errors.

The new system is not only more rapid in operation than the old one (fewer man hours required), but has consistently produced data of superior resolution while operating with a lower test power in resistors. A dc current-linkage balance is used to determine the standard-unknown differences while both are connected in series and totally immersed in a specially designed circular oil bath, which remains completely covered during all tests. Bath temperature is maintained constantly at  $25,000^\circ\text{C} (\pm 0.003^\circ\text{C})$  in a unique manner.

- 12516.** Yokel, F. Y., Somes, N. F., **Performance criteria for innovative housing systems**, *J. Am. Soc. Eng. Ed.* **61**, No. 2, 105-107 (Nov. 1970).

**Key words:** Building code; building systems; housing; performance criteria; performance testing.

A philosophy for the application of the performance concept to the evaluation of innovative housing systems is evolved, and its application to Operation BREAKTHROUGH is illustrated by examples.

- 12517.** Zalewski, E. F., Keller, R. A., **Tunable multiple wavelength organic-dye laser**, *Appl. Opt.* **10**, No. 12, 2773-2775 (Dec. 1971).

**Key words:** Dye laser; laser; organic dye laser; spectroscopy.



A technique for simultaneously tuning a dye laser at two different wavelengths has been developed. The apparatus consists of an optical cavity formed by two partially transparent, broad-band mirrors. A diffraction grating is placed along the optical axis outside of each mirror to form a secondary cavity. When the gratings are at the proper angle, there is enough optical feedback through the partially transparent mirrors to cause the laser to emit only at the wavelengths corresponding to the grating angles. Two wavelength outputs with each wavelength separately tunable were obtained from a rhodamine 6G organic dye laser using this technique.

**12518.** Andrews, J. R., **An interfacing unit for a 28 psec feedthrough sampling head and a random sampling oscilloscope**, *Rev. Sci. Instr.* **42**, No. 12, 1882-1885 (Dec. 1971).

**Key words:** GHz; impulse; picoseconds; random sampling; sampling head; sampling oscilloscope; spark-gap.

In time domain measurements of repetitive pulses there are situations when a signal delay line cannot be tolerated and a signal pretrigger is not available. In such situations, a random sampling oscilloscope system must be used. In the course of recent research activities, the author encountered the need to employ a remote, 50  $\Omega$  feedthrough, 28 psec transition time, wide-band sampling head with a random sampling oscilloscope system. Because the sampling head and the random sampling system were incompatible units from different manufacturers, an interfacing system was required to connect the two units. Presented here are a working design for the interface and operating results.

**12519.** Cashion, J. K., Mees, J. L., Eastman, D. E., Simpson, J. A., Kuyatt, C. E., **Windowless photoelectron spectrometer for high resolution studies of solids and surfaces**, *Rev. Sci. Instr.* **42**, No. 11, 1670-1674 (Nov. 1971).

**Key words:** High resolution electron energy analyzer; photoelectron spectroscopy; photoemission from solids and chemisorbed gases; ultrahigh vacuum; ultraviolet source.

An ultrahigh vacuum photoelectron spectrometer capable of measuring electron energy distributions for solids and chemisorbed gases at photon energies of 16.8, 21.2, 26.9, and 40.8 eV is described.

**12520.** Chang, S. S., Bestul, A. B., **Heat capacity and thermodynamic properties of *o*-terphenyl crystal, glass, and liquid**, *J. Chem. Phys.* **56**, No. 1, 503-516 (Jan. 1, 1972).

**Key words:** Calorimetry; configurational entropy; glass; heat capacity; *o*-terphenyl; residual entropy; viscosity; vitreous state.

The heat capacity of *o*-terphenyl has been measured with an adiabatic calorimeter for the crystal from 2 K to  $T_m$  (329.35 K), for the glasses from 2 K to  $T_g$  (around 240 K) and for the liquid from  $T_g$  to 360 K, on a sample with less than 0.005 mole % impurity. The heat of fusion and the entropy of fusion are 17 191 J mole<sup>-1</sup> and 52.20 J K<sup>-1</sup> mole<sup>-1</sup>, respectively. The residual entropy of the glasses at 0 K is about 15 J K<sup>-1</sup> mole<sup>-1</sup>. Above 170 K, the heat capacity of the *o*-terphenyl crystal is nearly proportional to the temperature to within 1%. Configurational entropy of the supercooled liquid, estimated from the result of this investigation, is used to relate the relaxation properties of glass-forming liquids according to the theory of Adam and Gibbs. Good agreement is found for both viscosity and NMR correlation frequency data.

**12521.** Cooper, J. W., Kolbenstvedt, H., **Differential energy and angular cross sections for ionization by several-hundred-keV electrons: Theory and comparison and experiment**, *Phys. Rev. A* **5**, No. 2, 677-687 (Feb. 1972).

**Key words:** Differential cross section; ionization; kilovolt electrons; Møller scattering.

A procedure for calculating cross sections for ionization of electrons in various shells of an atom differential in both angle and final electron energy is developed. Calculations for ionization of carbon, copper, and gold for incident energies in the range 100-400 keV are presented and compared with recent experimental results.

**12522.** Dalke, J. L., **International standards for magnetic materials and components**, *IEEE Trans. Magnetics* **MAG-7**, No. 3, 545-548 (Sept. 1971).

**Key words:** IEC; international standards; magnetic components; magnetic materials; magnetic measurements; magnetic standards.

In practically all of the industrially developed countries of the world there are strong national standards organizations. The International Electrotechnical Commission (IEC) coordinates and unifies electrical and electronic standards by drafting international recommendations from which member countries may draw for national standards. The benefits derived from this work include better understanding among electrical and electronic engineers and scientists, and a means for initiating and expanding international trade. The upsurge in development and application of ferrites led the IEC to establish a committee on ferromagnetic oxide parts 15 years ago, which rapidly expanded into a full technical committee on magnetic materials and components (TC 51). The magnetic activities include recommendations for terms and definitions, dimensional standardization, measurement methods, inductors and transformers, data storage devices, strip-wound cores and laminations, variability (temperature and time), gyromagnetic applications (microwave), and antenna rods. Eleven TC 51 IEC publications are now available. Numerous others are in process.

**12523.** Daney, D. E., **Thermal conductivity of solid argon, deuterium, and methane from one-dimensional freezing rates**, *Cryogenics* **11**, No. 4, 290-297 (Aug. 1971).

**Key words:** Instrument; solid argon; solid deuterium; solidified gases; solid methane; thermal conductivity.

The thermal conductivities of solid argon, deuterium, and methane have been determined near their triple points from measurements of one-dimensional freezing rates. In this new technique, a cylinder of liquid is frozen axially from one end, and the thermal conductivity of the freezing solid is evaluated from the freezing rate and the cylindrical cell end temperatures. A plastic cell wall offers the advantages of visual observation of the freezing solid and negligible cell wall conduction. The estimated random and systematic errors for the apparatus are 5 and 3%, respectively. Improved instrumentation may reduce these errors by one-half.

**12524.** de Graaf, L. A., Mozer, B., **Structure study of liquid neon by neutron diffraction**, *J. Chem. Phys.* **55**, No. 10, 4967-4973 (Nov. 15, 1971).

**Key words:** Correlation function; interatomic potential; neutron diffraction; structure factor.

Neutron-diffraction measurements with high statistical accuracy were performed on liquid neon at 35.05 K and at three different densities. The structure factors  $S(\kappa)$ , measured to momentum transfers  $\kappa$  of 13.2 Å<sup>-1</sup>, show a density-dependent structure well beyond 6 Å<sup>-1</sup>. The data have been used to calculate the radial distribution functions  $g(r)$ , the direct correlation functions  $c(r)$ , and effective interatomic potentials.

**12525.** Diller, D. E., **The specific heats ( $C_p$ ) of dense simple fluids**, *Cryogenics* 11, No. 3, 186-191 (June 1971).

Key words: Density dependence; molecular dynamics; simple fluids; specific heats; temperature dependence.

This paper examines the wide-range temperature and density dependences of the specific heats ( $C_p$ ) of a number of simple fluids (helium, neon, argon, krypton, parahydrogen, oxygen, and fluorine). The temperature range between the triple point and  $2T_c$  at densities up to  $3\rho_c$  is emphasized. The behaviour of the internal specific heats of the classical monatomic fluids is compared with that of the diatomic and quantum fluids and with internal specific heats derived from molecular dynamics calculations. This comparison shows that (to a first approximation) the internal specific heats of classical monatomic fluids depend only on the intermolecular pair potential energy.

**12526.** Domalski, E. S., **Evaluating experimental data on heats of combustion**, *J. Chem. Doc.* 11, No. 4, 234-237 (1971).

Key words: Bomb calorimetry; corrections to the combustion data; data evaluation; evaluation process; flame calorimetry; heats of combustion of organic compounds; recommendations to authors.

The approach used by data evaluators at the Chemical Thermodynamic Data Center of the National Bureau of Standards for the interpretation of published articles reporting values of the heats of combustion is discussed. An appropriate set of corrections is applied to the values when required to bring all data under study to a common base. Corrections which must be considered are: changes in calibration, reduction of the sample mass to vacuum, changes in atomic mass, reduction to standard states, expression of the data in proper energy units, and bringing the reference temperature for the combustion process to 298.15 K. Some corrections must be estimated because insufficient information is given in the article for a standard reanalysis. Guidelines are offered to authors of papers which will provide a maximum amount of data for the reexamination of experimental results, but yet maintain conciseness in the overall presentation.

**12527.** Eisenhart, C., **Youden's burette experiment**, *J. Quality Technol.* 4, No. 1, 20-23 (Jan. 1972).

Key words: Accuracy; analysis of variance; measurement process; precision; regression line; scheduling measurements; statistical design of experiments; systematic error; Youden's burette experiment.

This is a write-up of a lecture given by Dr. W. J. Youden at the National Bureau of Standards in 1947 which may be said to have had three objectives: first, to lay bare the fallaciousness of the all-too-common belief that statistical methods—and a statistician!—can be of no help unless one has a vast amount of data; second; to demonstrate that one can obtain valuable information on the precision—and even on the accuracy!—of a measurement process without making a large number of measurements on any single magnitude; and third, to show how in routine work one can often obtain useful auxiliary information on personnel, equipment, etc., at little or no additional cost, by skillful preliminary planning of the measurements to be taken. These precepts are demonstrated by an experiment involving only 8 volumes of liquid drawn from a burette by two different operators and subsequently subjected to chemical analysis by the same individuals.

**12528.** Ellerbruch, D. A., **Microwave methods for cryogenic liquid and slush instrumentation**, *IEEE Trans. Instr. Meas.* IM-19, No. 4, 412-416 (Nov. 1970).

Key words: Cryogenic fluids; densitometer; flowmeter; instrumentation; microwave.

Microwave instrumentation is being developed to measure densities and flow rates of nitrogen or hydrogen in either the single-phase liquid state or the liquid-solid (slush) state. The dielectric behavior exhibited by these fluids is the basis for using microwave systems for the measurement. These methods can also be applied to the measurement of fluids at ordinary temperatures.

The three density instrumentation techniques discussed here require that the microwave signal be propagated through a column of cryogenic fluid (from the top to the bottom of a cryostat, for example). All of the fluid in the column influences the behavior of the microwave signal, thus the sample is representative of the fluids at all levels within the cryostat.

A Doppler flowmeter is also discussed. Its main advantages are that no moving mechanical parts are involved and no probe need be installed in the flow stream. The flowmeter may give simultaneous density and velocity measurements so that the mass flow rate can be determined.

**12529.** Evenson, K. M., Day, G. W., Wells, J. S., Mullen, L. O., **Extension of absolute frequency measurements to the cw He-Ne laser at 88 THz (3.39  $\mu$ )**, *Appl. Phys. Letters* 20, No. 3, 133-134 (Feb. 1, 1972).

Key words: CO<sub>2</sub> laser; helium neon laser; laser frequency measurement; MOM diode; 3.39  $\mu$ m laser.

The highest absolute frequency measurement yet reported is described. The frequency of the 3.39- $\mu$  line from a He-Ne laser oscillating at the methane absorption frequency was found to be 88.376245 (55) THz. The frequency was measured by beating the 88-THz radiation with the R(30) line from a cw CO<sub>2</sub> laser and a 48-GHz klystron in a tungsten-on-nickel point-contact diode. The speed of light calculated from this frequency and previous wavelength measurements is in agreement with the accepted value and of comparable accuracy.

**12530.** Fatiadi, A. J., Schaffer, R., **Periodic acid as a new oxidant for the degradation of bile pigments. Isolation of a biliverdine type of reaction intermediate on oxidation of bilirubin with periodic acid**, *Experientia* 27, No. 10, 1139-1141 (Oct. 15, 1971).

Key words: Acid; bile; bilirubin; biliverdine; charge-transfer; complex; degradation; iodine; methyl-sulfoxide; periodic; pigment; structure.

Degradation of porphyrins and bile pigments can be performed with aqueous periodic acid by use of methyl sulfoxide, acetic acid, or tetrahydrofuran as the co-solvent. By the use of methyl sulfoxide as the co-solvent in the oxidation of bilirubin with periodic acid, it was possible to isolate a biliverdine-iodine complex to which a charge-transfer structure has been assigned.

**12531.** Fey, L., **Time dissemination capabilities of the Omega system**, *Proc. 25th Annual Frequency Control Symp., Atlantic City, N. J., Apr. 26-28, 1971*, pp. 167-170 (Electronic Industries Association, Washington, D.C., Apr. 1971).

Key words: Multiple frequency timing; Omega time code; precise time receiver; precise timing; time code receivers; VLF timing.

The Omega VLF navigation system affords an opportunity to disseminate time synchronization signals which could serve two classes of users: those who need precise timing and those who need time-of-day information in the form of a time code. This paper discusses precise timing use in terms of carrier pulse timing, multiple frequency techniques for carrier cycle ambiguity resolution, and Omega system capabilities in the microsecond region. For use where unattended automatic timing is needed, a



time code giving second, minute, hour, and day number information could serve a variety of needs. These are described along with characteristics and constraints of such a code imposed by the existing navigation format. The paper concludes with desirable receiver characteristics and development requirements for these two timing uses.

**12532.** Fickett, F. R., **Aluminum. 1. A review of resistive mechanisms in aluminum**, *Cryogenics* **11**, No. 5, 349-367 (Oct. 1971).

**Key words:** Aluminum; electron scattering; magnetoresistivity; resistivity; superconductivity.

Various mechanisms affecting the electrical resistivity of aluminum are reviewed. Brief treatments are given of the theory, experimental techniques, and the results of experiments to measure the effect of phonons, electron-electron interactions, boundaries, vacancies and interstitials, chemical impurities, dislocations, and stacking faults on the resistivity of aluminum at room temperature and below. Also reviewed are experimental data on superconductivity, magnetoresistivity, and the effect of interactions between the various mechanisms. Where appropriate, suggested values are given for the resistivity contribution of a particular mechanism.

**12533.** Foote, W. J., **A new flange design for O-ring seals**, *Rev. Sci. Instr.* **41**, No. 8, 1237 (Aug. 1970).

**Key words:** Flange design; O-ring; seal; vacuum.

A new type of O-ring seal was designed to provide a vacuum-tight cover for a wide-mouth cylindrical dewar. Covers using this type of seal are cheaper to machine than conventional designs, and can be quickly installed or removed. The design may be used to vacuum seal almost any smooth walled cylindrical vessel or large tubing.

**12534.** Giarratano, P. J., Arp, V. D., Smith, R. V., **Forced convection heat transfer to supercritical helium**, *Cryogenics* **11**, No. 5, 385-393 (Oct. 1971).

**Key words:** Correlations; cryogenics; forced convection; heat transfer; helium; supercritical.

Heat transfer coefficients have been measured for supercritical helium, circulated around a closed flow loop by a miniature centrifugal pump. Reynolds numbers in the 0.208 cm i.d. by 10 cm long stainless steel test section ranged from  $1 \times 10^4$  to  $3.8 \times 10^5$  with pressures 3 to 20 atm (0.3 to 2 MN/m<sup>2</sup>) and fluid temperatures 4.4 to 30 K. Wall-to-bulk temperature ratios varied from approximately 1.03 to 3.0. Results indicate an enhancement in heat transfer as the bulk temperature of the fluid approaches the transposed critical temperature. This improvement is qualitatively predicted by classical correlations due to the increase of thermal conductivity and specific heat in this region. Over the range of variables included in the measurements it was found that a modification of the Dittus-Boelter heat transfer correlation can be used to predict the heat transfer coefficient satisfactorily for most engineering calculations.

**12535.** Guttman, C. M., **Low-temperature heat-capacity differences between glasses and their crystals**, *J. Chem. Phys.* **56**, No. 1, 627-630 (Jan. 1, 1972).

**Key words:** Crystals; disordered crystal; glasses; heat capacity; low temperature.

It is suggested that the low-temperature heat-capacity difference between glasses and their crystal may be computed by considering the simple process,  $C_x(V_x) \xrightarrow{\partial/\partial V} C_x(V_g) \xrightarrow{\partial/\partial T} C_g(V_g)$ , where  $C_x(V_x)$  is the constant volume heat capacity of the crystal at its equilibrium volume at normal pressures,  $V_x$ ,  $C_x(V_g)$  is the heat capacity of the substance of identical structure as the crystal

but of a volume,  $V_g$ , equivalent to that of the glass, and  $C_g(V_g)$  is the constant volume heat capacity of the glass. Estimates are made of the change in heat capacity due to step (a) (the change in heat capacity at constant crystal structure due to a volume change) and to step (b) (the change in heat capacity due to disordering at constant volume) for a one-dimensional model of a glass and crystal. These suggest that step (a) contributes more to the heat-capacity difference than does step (b). Contributions to step (a) from a three-dimensional Debye model show reasonable agreement with experiment.

**12536.** Hanson, D. W., Hamilton, W. F., **One-way time synchronization via geostationary satellites at UHF**, *IEEE Trans. Instr. Meas.* **IM-20**, No. 3, 147-153 (Aug. 1971).

**Key words:** Clocks; delay; ranging measurements; satellites; synchronization; timing; UHF.

This paper describes an experiment designed to evaluate the accuracy of one-way clock synchronization using geostationary satellites with the propagation delays calculated from the satellite's orbital elements. Propagation delays from a ground transmitter via satellite to each of five locations in the North and South American continents were measured and compared with the calculated values. Three months of data are presented along with descriptions of the equipment, timing signal format, and methods for delay calculation and time recovery.

The results show that within two weeks of epoch for the orbital elements, clocks can be synchronized to 150  $\mu$ s using the Tactical Communications Satellite (TACSAT). If one of the observers of the timing signals was already synchronized to the master clock, his delay measurement could improve the results for TACSAT to 75  $\mu$ s. By the same method and within 12 hours of epoch, the results for the Lincoln Experimental Satellite-6 (LES-6) indicated that synchronization to 25  $\mu$ s was possible.

**12537.** Heinrich, K. F. J., **Errors in theoretical correction systems in quantitative electron probe microanalysis—a synopsis**, *Anal. Chem.* **44**, No. 2, 350-354 (Feb. 1972).

**Key words:** Electron probe microanalysis; errors; fluorescence; iteration; x-ray absorption; x-ray emission.

Accurate electron probe microanalysis with simple reference materials requires the use of theoretical models describing the emission of direct and indirect characteristic x-radiation, and of an iterative calculation procedure. The presently accepted theoretical equations for the calculation of intensities are presented, with discussion of the main sources of error. An efficient iteration procedure which uses a hyperbolic approximation to the analytical calibration curve is discussed in detail.

**12538.** Hust, J. G., Clark, A. F., **The Lorenz ratio as a tool for predicting the thermal conductivity of metals and alloys**, *Mater. Res. Stand.* **11**, No. 8, 22-24 (Aug. 1971).

**Key words:** Alloys; cryogenics; electrical resistivity; electron conductivity; Lorenz ratio; low temperature research; metals; thermal conductivity; thermal resistance.

From a knowledge of the Lorenz ratio of a given class of alloys and a simple electrical resistivity measurement, one can calculate the thermal conductivity of a specimen with reasonable accuracy. A discussion contrasts the characteristic temperature dependence of the Lorenz ratios,  $\rho\lambda/T$  ( $\rho$  = electrical resistivity,  $\lambda$  = thermal conductivity,  $T$  = temperature), of metals and alloys with high conductivity with that of metals and alloys with low conductivity. An additional classification of alloys in terms of Lorenz ratio further enhances the predictive capabilities of the method. The advantages as well as the limitations of the method are discussed.

12539. Jennings, D. A., Varga, A. J., Efficient second harmonic generation in ADP with two new fluorescein dye lasers, *J. Appl. Phys.* **42**, No. 12, 5171-5172 (Nov. 1971).

Key words: ADP crystals; dye laser; fluorescein dye; second harmonic generation; tunable UV source.

Two new fluorescein solutions for flashlamp-pumped dye lasers are reported, providing peak powers on the order of kilowatts, tunable from 550 to 580 nm. The 90° phase-matched second harmonic generation in ADP demonstrated with these and other dyes provides a flash excited UV source tunable from 250 to 290 nm with peak powers of about 10 watts.

12540. Kestin, J., Paykoc, E., Sengers, J. V., On the density expansion for viscosity in gases, *Physica* **54**, 1-19 (1971).

Key words: Argon; dense gases; helium; nitrogen; transport properties; viscosity.

The paper presents the results of new, precise measurements of the viscosity of nitrogen, argon, and helium at 25 °C. The measurements were performed over a nominal range of pressures 1-100 atm and at very closely spaced density intervals. The data were subjected to a stringent statistical analysis in order to determine whether the density expansion consists of a pure polynomial or whether a term of the form  $\rho^2 \ln \rho$  must be included in it. The existence of such a term was discovered theoretically by several investigators. The analysis indicates that if such a term exists, its factor must be very small. Moreover, the statistically significant interval of values which this factor can assume includes zero in it.

This result is interpreted as indicating that correlations which extend over distances of the order of a mean free path are negligible when compared with correlations which extend over distances of the order of the range of molecular interactions.

12541. Koonce, C. S., Mangum, B. W., Thornton, D. D., Magnetic properties of the antiferromagnet  $\text{DyPO}_4$  in applied fields, *Phys. Rev. B* **4**, No. 11, 4054-4069 (Dec. 1, 1971).

Key words: Antiferromagnet; dipolar interactions;  $\text{DyPO}_4$ ; heat capacity; magnetization; metamagnet; phase transition; shape effects; susceptibility.

The magnetization and susceptibility of the Ising antiferromagnet  $\text{DyPO}_4$  have been measured as a function of temperature and applied field for samples having demagnetization factors  $D \approx 0.02$  and  $D \approx 1.0$ . Also, the temperature at which peaks in the heat capacity at constant applied field occurred were measured for a number of applied fields. These results have been compared with predictions of the molecular-field approximation and the Bethe-Peierls approximation including long-range dipolar interactions. The temperature below which the antiferromagnetic-paramagnetic transition is first order has been obtained within the molecular-field approximation. In addition, expressions are obtained for the magnitude of the discontinuity in the heat capacity at the transition between the intermediate (or mixed) state and the antiferromagnetic or paramagnetic states for samples having nonzero demagnetization factors. These expressions do not depend on the molecular-field or Bethe-Peierls approximations.

12542. Kuriyama, M., X-ray Compton-Raman scattering, *Acta Cryst.* **A27**, Part 6, 634-647 (Nov. 1971).

Key words: Absorption; charge correlation; Compton effect; core electrons; current correlation; inelastic scattering; solid; theory; valence electrons; x-ray Raman effect.

X-ray Compton-Raman scattering is reviewed from an original point of view. The differential cross section for x-ray inelastic scattering from crystals is derived from first principles to explain

the coexisting Compton and Raman scattering in solids. This derivation makes it possible to express the cross section in terms of the current correlation of electrons in a crystal. All the electrons, including the core electrons, are treated on an equal basis in this formulation. The relationship between the x-ray absorption spectrum and the inelastic scattering spectrum is discussed in detail. This formulation provides a theoretical justification to the importance of x-ray inelastic scattering experiments in connection with an experimental determination of the two-particle Green's function. In the Appendices the theoretical formulations are given in detail, which apply not only to the ordinary inelastic scattering process, but also to the processes involving Bragg diffraction.

12543. Kushner, L. M., Technology, product performance, and the consumer, *Sci. Teacher* **38**, No. 8, 22-26 (Nov. 1971).

Key words: Product performance; technology; technology assessment.

The relationship between technology and the consumer is a complex one. Its most obvious manifestation is in the performance of the products he purchases; but one must also take into account the impact of technology on the manufacturing process and on the buying habits of the consumer. The overriding effect of technological advance, however, has been to put the consumer very much at a disadvantage relative to his former position as an equal in face-to-face bartering with an individual craftsman. The courts, through an increasingly strict view of manufacturer liability, and the Congress, through its consideration of a host of consumer protection bills, are attempting to redress this imbalance. Responsible business and industry are seeking, through the voluntary standardization process to improve the situation; but this process, developed to suit the industrial buyer and seller, appears to be ill-suited to the task without substantial modification. As with the other serious and intricate problems society faces today, there are no simple solutions but to the extent that the consumer begins to understand his situation vis-a-vis technological development he becomes better able to deal with it. This is one of the challenges facing the educational community in general and science teachers in particular.

12544. Maki, A. G., A high resolution study of *l*-type resonance in cyclopropane, *J. Mol. Spectrosc.* **41**, No. 1, 177-181 (Jan. 1972).

Key words: Cyclopropane; energy levels; infrared; *l*-type resonance; molecular structure; spectroscopy.

The  $\nu_5 + \nu_{10}$  band of cyclopropane ( $\text{C}_3\text{H}_6$ ) centered at  $2089.52 \text{ cm}^{-1}$  has been measured and analyzed taking into account the *l*-type resonance effect described by Cartwright and Mills. A least-squares fit of more than 300 well-resolved transitions gave a set of band constants which reproduced the measurements with a standard deviation of  $0.003 \text{ cm}^{-1}$ . The analysis confirms the *l*-type resonance treatment given by Cartwright and Mills and shows that their band contour fit gave remarkably accurate constants for this band.

12545. Mann, D. B., Cryogenic flow-metering research at NBS, *Cryogenics* **11**, No. 3, 179-185 (June 1971).

Key words: Cryogenic-fluid-flow measurement; cryogenic flowmetering; liquid argon; liquid nitrogen.

One very pressing cryogenic problem is that of cryogenic fluid flow measurement. An NBS programme, which focuses attention on the problem, has as its objectives to (1) establish present state-of-the-art by evaluating existing measurement methods, (2) establish methodology to maintain precision and accuracy of field-measurement devices, and (3) establish a comprehensive programme to develop new cryogenic fluid-measurement



systems. The scope of this programme includes a precision measurement capability for measuring the flow of liquid nitrogen and liquid argon, a transfer of technology from the traditional cryogenic fluids to measuring the flow of liquefied natural gas and methane, and a concerted effort to develop new mass-flow measurements for cryogenic fluids such as slush or liquid hydrogen. Cryogenic flow-metering history is given as well as a description of three flow facilities that establish experimental confirmation of the cryogenic flow-measurement system under investigation.

**12546.** Mighell, A. D., Santoro, A., **The crystal and molecular structures of hexakis(imidazole) cadmium(II) nitrate,  $[\text{Cd}(\text{C}_3\text{H}_4\text{N}_2)_6](\text{NO}_3)_2$ , and hexakis(imidazole)cadmium(II) hydroxide nitrate tetrahydrate,  $[\text{Cd}(\text{C}_3\text{H}_4\text{N}_2)_6](\text{OH})(\text{NO}_3) \cdot 4\text{H}_2\text{O}$ , *Acta Cryst. B27*, Part 11, 2089-2097 (Nov. 1971).**

Key words: Cadmium; coordination complex; crystal structure; imidazole; x ray.

The crystal and molecular structures of hexakis(imidazole)cadmium(II) nitrate,  $[\text{Cd}(\text{C}_3\text{H}_4\text{N}_2)_6](\text{NO}_3)_2$ , and hexakis(imidazole)cadmium(II) hydroxide nitrate tetrahydrate,  $[\text{Cd}(\text{C}_3\text{H}_4\text{N}_2)_6](\text{OH})(\text{NO}_3) \cdot 4\text{H}_2\text{O}$ , have been determined by single-crystal x-ray diffraction techniques.  $[\text{Cd}(\text{C}_3\text{H}_4\text{N}_2)_6](\text{NO}_3)_2$  crystallizes in the trigonal system, space group  $R\bar{3}$ . The lattice parameters (hexagonal axes) are  $a = 12.633(2)$ ,  $c = 15.049(2)$  Å,  $Z = 3$ ,  $\rho_0 = 1.54$  g·cm<sup>-3</sup>,  $\rho_c = 1.54$  g·cm<sup>-3</sup>. The final three-dimensional full-matrix least-squares refinement resulted in an  $R$  value of 3.6% based on 1343 observed reflections.  $[\text{Cd}(\text{C}_3\text{H}_4\text{N}_2)_6](\text{OH})(\text{NO}_3) \cdot 4\text{H}_2\text{O}$  crystallizes in the hexagonal system, space group  $P6_3/m$ . The lattice parameters are  $a = 9.0376(8)$ ,  $c = 21.729(3)$  Å,  $Z = 2$ ,  $\rho_c = 1.45$  g·cm<sup>-3</sup>,  $\rho_0 = 1.44$  g·cm<sup>-3</sup>. The final three-dimensional full-matrix least-squares refinement resulted in an  $R$  value of 5.4% based on 996 observed reflections. Both structures consist of discrete  $\text{Cd}(\text{C}_3\text{H}_4\text{N}_2)_6^{2+}$  cations and  $\text{NO}_3^-$  anions but as a result of the presence of water molecules and  $\text{OH}^-$  ions in the hydroxide complex, the packing of the cations in the two structures is considerably different. The ligand imidazole molecules are coordinated through the pyridine type nitrogen atoms ( $\geq \text{N}$ ) to the  $\text{Cd}^{2+}$  ions with an average bond distance  $\text{Cd} \cdots \text{N}$  of 2.363 Å and they are hydrogen bonded through the pyrrole type ( $-\text{N}-\text{H}$ ) nitrogen atoms to the nitrate groups. However, to accommodate hydrogen bonding, there is considerable difference in the orientation of the imidazole rings in the two complexes. Specifically, each ring in one of the two complex cations is rotated, about the  $\text{Cd}-\text{N}(1)$  direction, approximately 130° with respect to its counterpart in the other cation. The bond distances and angles between the atoms of the imidazole molecules are practically identical in the two structures.

**12547.** Page, C. H., **The International System of Units (SI), *Phys. Teacher* 9, No. 7, 379-381 (Oct. 1971).**

Key words: Giorgi; IEC, MKSA, SI; units.

An elementary discussion of the SI and its development from the MKS system of Professor Giorgi and the IEC.

**12548.** Peterson, W. K., Beaty, E. C., Opal, C. B., **Measurements of energy and angular distributions of secondary electrons produced in electron-impact ionization of helium, *Phys. Rev. A* 5, No. 2, 712-723 (Feb. 1972).**

Key words: Electron scattering; helium; ionization; secondary electrons.

The energy and angular distributions of electrons produced in the ionization of helium by electrons with energies between 100 eV and 2 keV have been measured in a crossed-beam apparatus consisting of a fixed hemispherical energy analyzer and a rotata-

ble electron gun. Distributions of secondary electrons (those electrons departing with energies less than one-half that of the incident primary electrons) were obtained for a wide range of energies and for angles between 30 and 150° with respect to the direction of the incident primary electron beam. The observed angular distributions were significantly different from the results of two early electron-impact measurements; however, they agreed to the extent expected with more recent results and with similar proton-impact data. For secondary energies above about 50 eV and for primary energies greater than 300 eV, the energy distributions (the cross sections integrated over angle) were observed to be very nearly equal to the distribution given by the Mott formula for free-electron-free-electron scattering multiplied by the number of electrons in the target.

**12549.** Phelan, R. J., Jr., Mahler, R. J., Cook, A. R., **High  $D^*$  pyroelectric polyvinylfluoride detectors, *Appl. Phys. Letters* 19, No. 9, 337-338 (Nov. 1, 1971).**

Key words: Detector; infrared; polyvinylfluoride; pyroelectric.

Polyvinylfluoride plastic films exhibit a normalized detectivity,  $D^*$  (500 K, 1, 1), of  $3 \times 10^8$  cm Hz<sup>1/2</sup>/W. This value for the infrared-detector figure of merit is close to the highest available from other pyroelectric materials. A pyroelectric coefficient of 1 nC/cm<sup>2</sup>K was obtained from the optical response, and a material figure of merit of  $1.3 \times 10^{-9}$  C cm/J was determined.

**12550.** Powell, R. L., Wagner, P., **Irradiation effects on low temperature thermal and electrical conductivities of two graphites, *Carbon Letters to Editor* 8, 690-692 (1970).**

Key words: Electrical conductivity; graphite; neutron irradiation damage; thermal conductivity.

Experiments to determine the effect of radiation on the low temperature (6-100 K) thermal conductivities and electrical resistivities of two commercially available graphites have been performed. Two specimens of H4LM grade graphite with sample axes oriented parallel and perpendicular to the grain respectively and one specimen of Graph-i-tite G with the sample axis oriented parallel to the grain were used for the experiments. The specimens were irradiated in the core of the reactor at a power level of five megawatts for a total exposure of 120 megawatt-hours. Integrated neutron dose was computed to be  $1.73 \times 10^{18}$  nvt and total gamma  $3 \times 10^9$  rads. The irradiation treatment reduced the thermal conductivity by a factor of about eight at 100 K and was also effective in reducing the temperature coefficient of the thermal conductivity. Similarly, the irradiation caused an increase in the electrical resistivity.

**12551.** Proctor, T. M., Jr., **A passive analyzer for ultrasonic shear waves, *J. Acoust. Soc. Amer.* 50, No. 5, 1379-1381 (Nov. 1971).**

Key words: Multiwaveguide; shear wave analyzer; shear wave orientation; shear wave transducer.

A device has been developed which allows the determination of the direction of shear particle motion generated by a single transducer. The normal ways of determining shear motion are to use another crystal of known polarization or to know the crystallographic geometry. This device analyzes the shear motion by use of reflection modes in a multiwaveguide assembly. The shear motion can be related to the geometry of this waveguide assembly.

**12552.** Radebaugh, R., Siegwarth, J. D., **Anomalous thermal resistance between sintered copper powder and dilute He<sup>3</sup>-He<sup>4</sup> solutions, *Phys. Rev. Letters* 27, No. 12, 796-799 (Sept. 20, 1971).**

Key words: Copper; cryogenics; dilution refrigerator; helium-3-helium-4; Kapitza resistance; phonon-electron interaction; powder.

The thermal resistances between seven samples of sintered copper powder and a nearly saturated dilute  $\text{He}^3\text{-He}^4$  solution were measured between 14 and 200 mK. All samples showed the anomalously high thermal resistances seen in metal foils, and the values are in semiquantitative agreement with recent calculations of Seiden. Reproducibility of samples was found to be excellent and oxide layers formed at room temperature had no detectable effect.

**12553.** Radebaugh, R., Siegwarth, J. D., *Dilution refrigerator technology*, *Cryogenics* 11, No. 5, 368-384 (Oct. 1971).

Key words: Cryogenics; dilution refrigerator; Fermi-Dirac statistics; heat exchangers; helium-3; helium-4; liquid helium; mixtures; quantum fluid; thermodynamic properties.

This review discusses theoretical and practical developments concerning the  $\text{He}^3\text{-He}^4$  dilution refrigerator. Properties of  $\text{He}^3\text{-He}^4$  solutions are briefly discussed in terms of the weakly interacting Fermi-Dirac gas model and reused to calculate the behaviour of dilution refrigerators. The thermodynamic behaviour of the dilution process is first discussed, and then an analysis of various types of heat exchangers is presented. The use of nearly optimum heat exchangers, designed by the method outlined here, can significantly reduce the liquid volumes required and/or reduce the low temperature limit of the continuous dilution refrigerator. With smaller liquid volumes, the refrigerator can be cooled down and can reach thermal equilibrium more rapidly. Discussions of various practical considerations and recent developments in hardware are also included. Some suggestions for future work and speculations on trends are presented.

**12554.** Rasmussen, A. L., *Measurement of laser energy of linear components of polarization at 1.060  $\mu$* , *Rev. Sci. Instr.* 42, No. 11, 1590-1593 (Nov. 1971).

Key words: Laser calorimeter; laser energy; laser polarization; laser power; reflectivity measurement.

A double reflecting plate calorimeter [*Rev. Sci. Instrum.* 41, 1479 (1970)] was used to evaluate the energy components of a pulsed 1.060  $\mu$  neodymium laser light beam entering the calorimeter polarized parallel ( $E_H$ ) and perpendicular ( $E_V$ ) to a horizontal plane. The relationship between these components varied from  $E_H = 0.94 E_V$  to  $E_H = 1.25 E_V$ . Estimated error of  $E_H$  and  $E_V$  is 2.3%. As a check on the accuracy of polarization component measurements at 1.060  $\mu$ , an intercomparison of data was made between this calorimeter and an NBS liquid cell calorimeter. The agreement was about 0.2%.

**12555.** Reed, R. P., *Materials at low temperatures (a series of review papers). Introduction*, *Cryogenics* 11, No. 5, 347-348 (Oct. 1971).

Key words: Cryogenics; materials properties; survey.

We intend to present a number of review papers critically evaluating research on particular materials (for example, aluminum) or groups of materials (for example, composites) to assist in appraisal for cryogenic use. Well-qualified experts have been asked to contribute to this series during the next several years.

**12556.** Reed, R. P., Clark, A. F., Schramm, R. E., *Defect annealing (4 to 295 K) after martensitic phase transformation in an Fe-29 Ni alloy*, *Scripta Met.* 5, No. 6, 485-488 (June 1971).

Key words: Electrical resistivity; iron-nickel alloys; martensite; point defects.

An Fe-29 Ni alloy has been cooled from room temperature to 4 K and the electrical resistance measured on warming. On cooling the alloy transformed from austenite to martensite. By comparing the immediate isochronal resistivity to the temperature dependent martensite resistivity, the recovery profile is obtained. Results indicate that a very considerable number (about 0.5 at.%) of point defects are introduced during a martensitic transformation.

**12557.** Reimann, C. W., Zocchi, M., Mighell, A. D., Santoro, A., *Crystal and molecular structure of nitratobis-(2,2'-dipyridyl)-cobalt(III) hydroxide nitrate tetrahydrate*,  $[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{NO}_3)](\text{NO}_3)(\text{OH})\cdot 4\text{H}_2\text{O}$ , *Acta Cryst.* B27, Part 11, 2211-2218 (Nov. 1971).

Key words: Dipyridine and nitrate ligands; hydrogen bonding; monoclinic symmetry; octahedral coordination; transition metal-Co(III)-coordination complex.

The structure of nitratobis-(2,2'-dipyridyl)cobalt(III) hydroxide nitrate tetrahydrate,  $[\text{Co}(\text{C}_{10}\text{H}_8\text{N}_2)_2(\text{NO}_3)](\text{NO}_3)(\text{OH})\cdot 4\text{H}_2\text{O}$ , has been determined by single-crystal x-ray diffraction techniques. Crystals of this complex are monoclinic with  $a = 10.923(2)$ ,  $b = 15.998(4)$ ,  $c = 14.442(2)$  Å,  $\beta = 101.93(2)^\circ$ , space group  $C2/c$ ,  $\rho_c = 1.57 \text{ g}\cdot\text{cm}^{-3}$ ,  $\rho_o = 1.54 \text{ g}\cdot\text{cm}^{-3}$ , and  $Z = 4$ . The structure was solved by Patterson and Fourier methods. The cobalt atom is octahedrally coordinated by two molecules of 2,2'-dipyridyl and by a bidentate nitrate group. Water molecules, nitrate groups, and the hydroxide ions are involved in hydrogen bonds which extend continuously in the  $a$  and  $c$  directions. The final refinement of the structure by full-matrix anisotropic least-squares analysis resulted in an  $R$  value of 6.2%, based on 2995 observed reflections.

**12558.** Sharp, K. G., Coyle, T. D., *Synthesis and some properties of trifluoro(trifluoromethyl)silane*, *J. Fluorine Chem.-Short Communication* 1, 249-251 (1971).

Key words: Difluoroiodo(trifluoromethyl)silane; fluorine; fluoroalkylsilanes; silicon; silicon difluoride; trifluoro(trifluoromethyl)silane.

The simplest member of the perfluoroalkylfluorosilane series,  $\text{CF}_3\text{SiF}_3$  has been prepared in high yield from  $\text{CF}_3\text{SiF}_2\text{I}$  and has been definitively characterized. The compound decomposes at  $78^\circ$  to form  $\text{SiF}_4$ ,  $\text{C}_2\text{F}_4$ , and cyclo- $\text{C}_3\text{F}_6$ . The thermal lability of  $\text{CF}_3\text{SiF}_3$  can account for equivocal reports in the existing literature regarding synthesis from perfluoroalkyl halides and Si/Cu alloy at high temperatures.

**12559.** Schroeder, L. W., de Graaf, L. A., Rush, J. J., *Neutron diffraction study of the trigonal and cubic phases of NaSH*, *J. Chem. Phys.* 55, No. 11, 5363-5369 (Dec. 1, 1971).

Key words: Crystal structure; ion orientation; libration; neutron diffraction; phase transition; reorientation; sodium hydrosulfide.

Neutron diffraction powder patterns have been measured for the trigonal and cubic phases of NaSH at 296 and 379 K, respectively. Several possible models describing the orientations of the  $\text{SH}^-$  ion in the trigonal phase were compared with the experimental results. A model in which the  $\text{SH}^-$  ions are aligned along the trigonal axis gave the best agreement between calculated and observed structure factors. Thus the transition from the cubic to trigonal phase apparently results from the alignment of the  $\text{SH}^-$  ions along one of the cube diagonals which then becomes shorter than the other resulting in the less symmetric trigonal structure. Several structural models were also considered for the cubic phase. The isotropic, free rotator mode describing the  $\text{SH}^-$  orientations can be rejected in favor of a less randomly disordered model by comparison with preliminary neutron inelastic



scattering data. The limited diffraction data in this phase, however, do not enable a distinction to be made between disordered models. The preliminary inelastic scattering results also indicate that the librational frequencies of the  $\text{SH}^-$  ions are similar in both phases, but that reorientations of the  $\text{SH}^-$  ion between equivalent directions occur at a much faster rate ( $\sim 10^{12} \text{ sec}^{-1}$ ) in the cubic phase.

**12560.** Siegwarth, J. D., Radebaugh, R., Analysis of heat exchangers for dilution refrigerators, *Rev. Sci. Instr.* **42**, No. 8, 1111-1119 (Aug. 1971).

Key words: Cryogenics; dilution refrigerator; heat exchangers; helium-3; helium-4.

Numerical calculations of the behavior of dilution refrigerator heat exchangers are discussed and some results for both discrete and continuous exchangers are presented. It is shown that thermal conductance along the stream is negligible for a typical continuous exchanger of the coaxial tube type, but becomes a dominant feature of a typical discrete exchanger operating below about 50 mK and degrades the performance considerably. A simple design change can be made that reduces the conductance along the liquid and improves the performance of such an exchanger. A simple means of determining whether conductivity is important in either continuous or discrete exchangers is given.

**12561.** Sullivan, D. B., Resistance of a silicon bronze at low temperatures, *Rev. Sci. Instr.* **42**, No. 5, 612-613 (May 1971).

Key words: Alloy; bronze; magnetoresistance; resistance; temperature coefficient.

A specially prepared silicon bronze is shown to be quite insensitive to magnetic field and temperature change at liquid helium temperatures. The temperature coefficient of resistance is of the order of a few parts per million per degree over the range 2-10 K and the change in resistance at a flux density of 1 T ( $10^4$  G) is about 10 ppm.

**12562.** Tsang, W., Thermal decomposition of 3,4-dimethylhexane, 2,2,3-trimethylpentane, *tert*-butylcyclohexane, and related hydrocarbons, *J. Phys. Chem.* **76**, No. 2, 143-156 (1972).

Key words: Bond energy; cyclohexyl radical; 3,4-dimethylhexane; heats of formation; *n*-propyl radical; *s*-butyl radical; shock tube; *t*-butyl radical; thermal decomposition; 2,2,3-trimethylpentane.

3,4-Dimethylhexane, 2,2,3-trimethylpentane, and *tert*-butylcyclohexane have been decomposed in a single-pulse shock tube. Rate expressions for the main bond-breaking steps are:  $k(\text{sec-C}_4\text{H}_9\text{-sec-C}_4\text{H}_9 \rightarrow 2 \text{ sec-C}_4\text{H}_9) = 10^{16.34} \exp(-37,900/T) \text{ sec}^{-1}$ ;  $k(\text{sec-C}_4\text{H}_9\text{-tert-C}_4\text{H}_9 \rightarrow \text{sec-C}_4\text{H}_9 + \text{tert-C}_4\text{H}_9) = 10^{16.30} \exp(-36,400/T) \text{ sec}^{-1}$ ; and  $k(\text{tert-C}_4\text{H}_9\text{-c-C}_6\text{H}_{11} \rightarrow \text{tert-C}_4\text{H}_9 + \text{c-C}_6\text{H}_{11}) = 10^{16.31} \exp(-37,300/T) \text{ sec}^{-1}$ . They lead to  $\Delta H_{f,300}(\text{sec-C}_4\text{H}_9) = 55 \text{ kJ/mol}$  (13.2 kcal/mol),  $\Delta H_{f,300}(\text{tert-C}_4\text{H}_9) = 39 \text{ kJ/mol}$  (9.3 kcal/mol), and  $\Delta H_{f,300}(\text{c-C}_6\text{H}_{11}) = 66 \text{ kJ/mol}$  (15.8 kcal/mol). Rate expressions for the decomposition of all hydrocarbons formed from *sec*-butyl or cyclohexyl radicals and methyl, ethyl, isopropyl, *tert*-butyl, *tert*-amyl, allyl, 1-methylallyl, propynyl, and benzyl radicals have been calculated. Estimates are given for the rates of decomposition of hydrocarbons formed from *n*-propyl radicals and any of the compounds listed above. The accumulated single-pulse shock tube data can now give quantitative information on the initial cracking patterns of almost all aliphatic hydrocarbons. The  $A$  factors determined in this study provide striking confirmation for the earlier observation that this value, per C—C bond, for alkanes is a constant. On this basis, it appears that  $D(\text{tert-C}_5\text{H}_{11} - \text{H}) - D(\text{tert-C}_4\text{H}_9 - \text{H}) = 5.4 \text{ kJ/mol}$ ;  $D(\text{sec-C}_4\text{H}_9 - \text{H}) - D(i\text{-C}_3\text{H}_7 - \text{H}) = 3.5 \text{ kJ/mol}$ ;  $D(n\text{-C}_3\text{H}_7 - \text{H}) - D(\text{C}_2\text{H}_5 - \text{H}) \sim 1.5 \text{ kJ/mol}$ . The

absolute magnitude of the  $A$  factors are all at least a factor of 10 lower than expected. It is demonstrated that recent chemical activation and very low pressure pyrolysis studies support the shock tube results.

**12563.** Wiederhorn, S. M., Johnson, H., Effect of pressure on static fatigue of glass, *J. Amer. Ceram. Soc.—Discussions and Notes* **54**, No. 11, 585 (Nov. 1971).

Key words: Fracture; glass; high pressure; static fatigue; strength.

The static fatigue behavior of glass at elevated pressures was studied using fracture mechanics techniques. Stress time-to-failure data were obtained on three different glass compositions exposed to high pressure water, 7 kbar. The fracture behavior of glass in water was observed to be insensitive to pressure. It is suggested that this insensitivity resulted from compensating mechanisms in which the increase in fracture resistance arising from a positive activation volume for stress corrosion cracking is balanced by a decrease in fracture resistance due to increased hydroxyl ion concentration at the crack tip.

**12564.** Zimmerman, J. E., Frederick, N. V., Miniature ultrasensitive superconducting magnetic gradiometer and its use in cardiography and other applications, *Appl. Phys. Letters* **19**, No. 1, 16-19 (July 1, 1971).

Key words: Cardiography; gradiometry; instrumentation; Josephson effect; magnetocardiography; magnetometry; superconducting devices.

A portable magnetic gradiometer was built using an rf-biased point contact device as a sensor and a superconducting flux transformer 2.5 cm in diameter by 10 cm long to couple to the gradient of the external field. The instrument is limited by fluctuations which are probably associated with an uneven boiling of the cryogenic liquids and by environmental fluctuations in some locations. It is shown that the inherent sensitivity can be increased by an order of magnitude by increasing the bias frequency from 30 to 300 MHz. A possible use of the instrument as a magnetocardiograph in an unshielded environment was demonstrated.

**12565.** Zimmerman, J. E., Sensitivity enhancement of superconducting quantum interference devices through the use of fractional-turn loops, *J. Appl. Phys.* **42**, No. 11, 4483-4487 (Oct. 1971).

Key words: Instrumentation; Josephson effect; magnetometry; superconducting devices.

A new "fractional-turn" configuration for superconducting quantum interference devices provides enhanced sensitivity, with large loop area and low loop inductance. By operating the new configuration at optimum bias frequency (300 MHz or higher), inherent field sensitivities of  $10^{-15} \text{ T}$  ( $10^{-11} \text{ G}$ ) or better can reasonably be expected. The operational sensitivity of an instrument using such a device would probably be limited by externally generated noise in most applications. The configuration is readily adaptable to measurements of both diagonal and off-diagonal components of the field gradient.

**12566.** Andrews, J. R., Nahman, N. S., Electron-beam deflection in traveling-wave oscilloscopes, (Proc. 11th Symp. Electron, Ion, and Laser Beam Technology, Boulder, Colo., May 12-14, 1971), Chapter in *Record of 11th Symposium on Electron, Ion, and Laser Beam Technology*, pp. 141-146 (San Francisco Press, Inc., San Francisco, Calif., 1971).

Key words: Cathode ray tube; CRT; deflection; electron beam; GHz; oscilloscope; picosecond; slow-wave; traveling-wave.

A generalized electron-beam deflection theory is presented that is applicable to fast- or slow-wave deflection structures in traveling-wave oscilloscopes. The theory includes the deflection structure circuit properties and the electron beam dynamics. The results of experiments on two traveling-wave deflectors are presented: (1) a fast-wave rectangular transmission line, and (2) a slow-wave serrated rectangular transmission line. The theoretical and experimental results were correlated in the frequency and time domains. The rise times of the experimental traveling-wave oscilloscopes were in the range of 95 to 211 picoseconds (ps).

**12567.** Barnes, I. L., Garfinkel, S. B., Mann, W. B., Nickel-63: Standardization, half-life and neutron-capture cross-section, *Int. J. Appl. Radiat. Isotop.* **22**, 777-781 (1971).

Key words: Half-life; mass-spectrometry; micro-calorimetry; Ni-63 neutron capture cross-section; radioactivity standards.

Nickel-63 has been standardized for activity using the National Bureau of Standards' radiation balance and a calculated value for the average beta-particle energy. From the activity and isotopic abundance of nickel-63 in May 1968, the half-life has been calculated to be 100.07 years ( $\pm 2.0$  percent). The neutron-capture cross-section of nickel-63 has been found to be  $23 \pm 3$  barn.

**12568.** Beehler, R. E., Cesium atomic beam frequency standards: A survey of laboratory standards development from 1949-71, *Proc. 25th Frequency Control Annual Symp., Atlantic City, N.J., Apr. 26-28, 1971*, pp. 297-308 (Electronic Industries Association, Washington, D.C., 1971).

Key words: Atomic frequency standards; cesium beam frequency standards; laboratory cesium standards.

A review is presented of progress achieved in the development of cesium atomic beam frequency standards during the past 20 years, including both trends in design philosophy and actual performance achieved. The emphasis will be on laboratory-type cesium standards, in which attempts are made to optimize both accuracy and stability performance with lesser emphasis on such features as size and weight, environmental sensitivity, operational convenience, and cost. However, some comparisons are also made with commercially-developed cesium standards in order to emphasize various tradeoffs that are made for different applications. Up-to-date information is included on the current status of cesium standards being used or developed in various national standards laboratories throughout the world. Finally, some future trends in the development of improved laboratory cesium standards are discussed briefly.

**12569.** Bennett, H. S., Damage to ceramics from high intensity Q switched lasers, (Proc. Conf. on Ceramics in Severe Environments, North Carolina State University, Raleigh, N.C., Dec. 7-9, 1970), Chapter in *Materials Science Research*, W. W. Kriegel, ed., **5**, 537-546 (Plenum Publ. Corp., New York, N.Y., 1971).

Key words: Extrinsic damage; intrinsic damage; laser materials; surface damage; switched lasers; thermal stresses.

One important factor limiting the advance of high power laser technology is the failure of laser materials due to optically induced damage. Examples of surface damage, extrinsic damage produced by inclusions, and intrinsic bulk damage (beam trapping) are presented. A model to treat metallic inclusions which absorb an appreciable amount of incident laser radiation in glass laser rods is formulated and used to estimate thermal stresses and changes in refractive indices due to the thermal

stress field. The feasibility of optical techniques to detect incipient damage sites also is discussed.

**12570.** Branscomb, L. M., Taming technology, *Science* **171**, 972-977 (Mar. 12, 1971).

Key words: Environmental pollution; performance specifications; product performance; technology.

The public is frustrated with technology. Science, the father of technology, stands accused of failing the human society, while much of the frustration results from the failure of our social institutions to use wisely and distribute fairly the benefits of technology. The resolution of conflicts must come from a combination of research, of responsible private action, and astute public policy—all carried on within a rational framework.

**12571.** Branscomb, L. M., The U.S. Metric Study, *Sci. Teacher* **38**, No. 8, 58-62 (Nov. 1971).

Key words: International system (SI); measurement language; metric system.

The U.S. Metric Study showed conclusively that we have only two real alternatives in the face of rapidly increasing use of the metric system of measurement in the world and in this country: to convert to use of the metric system deliberately with a plan or to go metric eventually without a plan. It is plain that the American education system will have to improve its performance if we are to adjust, by whatever mechanism, to our increasingly metric world. It also appears that the metric system could be thoroughly introduced into the educational system at a relatively moderate cost.

**12572.** Broadhurst, M. G., Dielectric properties of methyl stearate-A model crystalline polymer, (Proc. Symp. Dielectric Properties of Polymers, American Chemical Society Meeting, Los Angeles, Calif., Mar. 30, 1971), Chapter in *Dielectric Properties of Polymers*, F. E. Karasz, ed., pp. 129-145 (Plenum Publ. Corp., New York, N.Y., 1972).

Key words: Crystalline polymers; dielectric measurements; dielectric relaxation; dynamical diffusion; Grüneisen constant; methyl stearate; pressure.

The dielectric properties of methyl stearate,  $\text{CH}_3 - (\text{CH}_2)_{16} - \text{C}=\text{O}-\text{O}-\text{CH}_3$ , have been measured as a function of pressure and temperature with special emphasis on the  $\alpha$  loss maxima. The experimental techniques are described and the frequency position, amplitude and width of the  $\alpha$  loss region are given at 213, 243 and 263 K and at 0, 1 and 2 kbars pressure. The activation parameters at  $P=0$  are  $\Delta H^\ddagger = 12.6$  kcal/mol,  $\Delta S^\ddagger = 20$  e.u.,  $\Delta V^\ddagger = 29$  cm<sup>3</sup>/mol and  $\log A = 16.4$ . The ratio of constant volume to constant pressure activation energy was found to be 0.85 and  $(\partial T/\partial P)_{f_{\max}} \approx 15$  °C/kbar. A general model suggested by the results is discussed, and a dynamical theory is presented which predicts the temperature, pressure, and chain length dependence of the relaxation frequency in terms of bulk thermodynamic functions. (1 kcal/mol = 4.184 kJ/mol, 1 e.u. = 4.184 J/mol-K, 1 kbar =  $10^8$  N/m<sup>2</sup>).

**12573.** Carpenter, B. S., Determination of trace concentration of boron and uranium in glass by the nuclear track technique, *Anal. Chem.* **44**, No. 3, 600-603 (Mar. 1972).

Key words: Boron; fission track counting; glass; neutron activation analysis; nuclear track technique; uranium.

The direct determination of boron and uranium was made on the National Bureau of Standards four trace element glass standards, nominally 500 ppm, 50 ppm, 1 ppm, and 0.02 ppm. The track counting results are compared with data obtained by isotope-dilution mass spectrometry. In addition the radial dis-



tribution of boron and uranium across the surface of the glass is discussed.

- 12574.** Carter, G. C., Bennett, L. H., <sup>115</sup>In Knight shifts in liquid alloys containing small amounts of Pb, *Phys. Rev. B* **5**, No. 5, 2022-2023 (Mar. 1, 1972).

Key words: Anisotropic scattering; In-Pb; Knight shift; liquid alloys; many body effects; nuclear magnetic resonance.

Measurements of the nuclear magnetic resonance of <sup>115</sup>In in very dilute Pb in In liquid alloys have been made. No structure was observed in the Knight shift vs composition behavior.

- 12575.** Cohen, G. G., Alexandropoulos, N. G., Kuriyama, M., Energy loss spectrum of lithium metal in the region of intermediate momentum transfer, *Solid State Commun.* **10**, 95-98 (Mar. 1972).

Key words: Collective excitations; energy transfer; lithium; momentum transfer; x-ray inelastic scattering.

An x-ray inelastic scattering spectrum of polycrystalline lithium with Cu-K $\alpha$  radiations was taken at the scattering angle 25° which corresponds to an intermediate momentum transfer ( $\kappa/k_f = 1.59$ ). The unfolded spectrum showed a steep fall-off on the large energy transfer side, indicating that individual excitations of electrons are suppressed strongly.

- 12576.** Collier, R. S., Jellison, J. C., Fluid-phase and temperature measurement with a single sensor. II, (Proc. 1970 Cryogenic Engineering Conf., June 17-19, 1970, Colorado Univ., Boulder, Colo.), Chapter in *Advances in Cryogenic Engineering*, K. D. Timmerhause, ed., **16**, Paper F-3, 251-260 (Plenum Press, Inc., New York, N.Y., 1971).

Key words: Fluid phase discrimination; hydrogen; low gravity; resistance thermometer; thin carbon film.

A method is described for obtaining fluid phase and temperature measurement of hydrogen with a single sensor. The sensor is a 1/8-inch diameter, 3/4-inch long sapphire cylinder on which is deposited a thin carbon film which is stable on thermal cycling and sensitive as a resistance thermometer in the temperature range 4-300 K. The sensor is pulsed with an electrical power input and a fluid phase discrimination (FPD) circuit samples the transient response of the sensor. This transient is a function of the sensor being in liquid or gas. The sensor returns to equilibrium between power pulses and a temperature measurement is taken at the onset of the next power pulse. This dual measuring process can occur at a sample rate of 20 Hz.

A drop tower experiment is described which demonstrates the utility of these sensors in a dynamically changing situation. The sensor response time as the sensor goes from gas to liquid is 50 milliseconds (one sample time); the response time from liquid to gas varies from 50 milliseconds to 1.2 seconds in normal gravity and from 50 milliseconds to 3.0 seconds in low gravity.

- 12577.** Colson, J. P., Eby, R. K., Sinnott, K. M., Alpha relaxation in polyethylene, *J. Appl. Phys.* **42**, 13, 5902-5903 (Dec. 1971).

Key words: Alpha; density; lamella thickness; polyethylene; relaxation; solvent; unit cell.

It has been shown previously that the strength and temperature (peak) of the relaxation in solution-grown crystals of polyethylene appear to correlate with a number of parameters including lamella thickness, unit-cell dimensions, density, and residual solvent content. However, it has been reported also that in two samples which had different thermal histories for which all the above parameters are equal, the strength of the relaxation was the same but the temperature of the relaxation peak differed

by 15 °C. It is the purpose of this communication to confirm this observation and to report that the difference in relaxation temperature decreases with increasing annealing temperature and becomes zero at 130 °C, while the above parameters remain equal in the two samples.

- 12578.** Colson, J. P., Reneker, D. H., Electron irradiation effects in polyoxymethylene crystals grown inside trioxane crystals, C. J. Arceneaux, ed., *29th Annual Proc. Electron Microscopy Society America, Boston, Mass.*, pp. 78-79 (1971).

Key words: Polyoxymethylene crystals; trioxane crystals.

Polyoxymethylene (POM) crystals grow inside trioxane crystals which have been irradiated and heated to a temperature slightly below their melting point. Detailed examination at higher magnification showed that three distinct types of POM crystals grew in a typical sample. We have observed the sensitivity of each type of crystal to irradiation with 80 kilovolt electrons.

- 12579.** Corliss, E. L. R., Berendt, R. D., Computers—A white collar hazard, *Pollut. Eng.* pp. 27-30 (Jan.-Feb. 1972).

Key words: Computer noise; damage-risk criteria; hearing loss; noise control; scanning analyzer; spectral distribution.

Noise levels generated by modern computers are high enough in some circumstances to induce hearing loss. Attention was recently focused on noise problems in computer laboratories because of the relatively simple and recurrent errors made by programmers possibly as a result of distraction induced by the very high noise levels under which they were working. It turned out, however, that the first order of business proved to be the protection of hearing itself.

- 12580.** Costrell, L., An introduction to CAMAC, *CAMAC Bull.* Issue No. 2, 3-6 (Nov. 1971).

Key words: CAMAC; computer interfacing; control systems; instrumentation; instrumentation standards; nuclear instrumentation; standards.

The CAMAC instrumentation system developed by the ESONE Committee of European Laboratories has been endorsed by the U.S. AEC NIM Committee as a dataway system complementary to the NIM (Nuclear Instrument Module) system. CAMAC is described in a general way in this condensed version of the introductory paper of the CAMAC Tutorial Session of the 1970 IEEE Nuclear Science Symposium.

- 12581.** Crissman, J. M., Passaglia, E., Internal-friction study of high-purity single crystals of *n* eicosane (C<sub>20</sub>H<sub>42</sub>), *J. Appl. Phys.* **42**, No. 12, 4636-4644 (Nov. 1971).

Key words: Cold-work; dislocation relaxation; internal friction; *n*-alkane; relaxation process; Young's modulus.

Large pure single crystals of *n* eicosane (C<sub>20</sub>H<sub>42</sub>) with [210] growth axes have been prepared by slow crystallizations from the melt. Internal-friction measurements covering temperatures from 100 to 300 K at  $\approx 1$  kHz reveal that in the as-grown single crystals both the  $\alpha$  and  $\gamma$  loss peaks characteristic of polycrystalline *n* alkanes of less purity are absent, from which we conclude that, in polycrystals, these processes are a result of impurities and/or crystal defects. Two very weak loss maxima of obscure origin were observed at about 270 and 287 K for all the crystals studied. In one single crystal progressive stages of light cold work induced a complex spectrum of small loss maxima between 200 and 300 K. These maxima were found to be highly sensitive to aging. We believe that the observed behavior provides evidence for dislocation motion in crystals of this type. No detectable  $\gamma$  peak resulted from the cold work. Data are also included for one single crystal which was irradiated with  $\gamma$  rays.

**12582.** Cuthill, J. R., **Satellites in soft x-ray spectra**, J. Thewlis, ed., *Encyclopaedic Dictionary of Physics* **4**, 1-2 (1971).

Key words: Auger transition; Coster-Kronig theory; non-diagram lines; Wentzel theory; x-ray satellite lines.

"Satellites" in soft x-ray spectra are defined. The transitions responsible for some common satellite lines are discussed.

**12583.** Cuthill, J. R., **Soft x-ray spectroscopy**, J. Thewlis, ed., *Encyclopaedic Dictionary of Physics* **4**, 1-11 (1971).

Key words: Absorption spectra; electron transitions; emission spectra;  $L_{2,3}$  emission spectra; shells; soft x-ray spectroscopy; valence bands.

The soft x-ray range is not precisely defined but for practical purposes can be said to begin where an air or helium path and conventional windows cannot be used and extends up to where the techniques of optical spectroscopy are applicable (approximately 2.5 to 500 Å). Solid state x-ray emission spectra in this range involve electron transitions from the valence band into one of the outermost normally full shells. The corresponding absorption spectra involve transitions from one of the outermost normally full shells to available empty states in the conduction band. The emission and absorption spectra are thus a measure of the density of occupied and unoccupied states, respectively, in the valence band. Examples of the interpretation of metal and alloy spectra in relation to bonding and density of states are given. In light elements ( $Z < 10$ ) analysis by x-ray spectroscopy the K spectrum is the valence band spectrum and spectrochemical analysis loses its unique feature of being independent of the state of chemical combination. The changes in shape and the shifts in the peaks and edges in the emission band spectra that take place as a result of alloying now have to be taken into account in chemical analysis.

Another important application of soft x-ray spectroscopy is to the study of the radiation due to the recombination of highly ionized atoms in a plasma. An interesting example is the corona of the sun. Examples of some of the first soft x-ray spectra obtained of the sun's corona during solar flares, which are by means of satellite mounted spectrometers, are given.

Instrumentation for the soft x-ray range is described.

**12584.** Davis, D. D., Blair, B. E., Barnaba, J. F., **Long-term continental U.S. timing system via television networks**, *IEEE Spectrum* **8**, No. 8, 41-52 (Aug. 1971).

Key words: Atomic clock comparisons; clock comparisons; Loran-C; NBS time scale; portable clocks; time synchronization; TV timing; USNO time scale.

Hundreds of atomic frequency standards and precision crystal oscillators exist in remote locations throughout the continental U.S. that are synchronized through fairly complex and costly means. Today, however, an inexpensive synchronization system is available in the form of live television broadcasts by commercial networks. In precision and accuracy, the television method is comparable to the portable atomic clock and/or Loran-C, with average day-to-day differential delays less than 1  $\mu$ s. Based on the results of the tests presented here, the use of nearly any solid-state television receiver and a low-cost horizontal sync pulse generator can provide 10- $\mu$ s synchronizations at all times. The operation of a TV line-10 timing system, including the circuitry of auxiliary equipment, is also included. This article gives about 1 1/2 years of substantiating data for the three major commercial networks (ABC, CBS, and NBC). There is also provision for synchronization with the NBS and/or USNO Coordinated Universal Time (UTC) scales through regularly published reports.

**12585.** Deason, V. A., Clark, A. F., Powell, R. L., **Characterization of high purity metals by the residual resistivity ratio**, *Mater. Res. Stand.* **11**, No. 8, 25-28 and 52 (Aug. 1971).

Key words: Contaminants; cryogenics; eddy currents; eddy current tests; electrical resistivity; nondestructive tests; purity; scattering; time constant.

In recent years the residual resistivity ratio has been widely used as a sensitive indicator of chemical purity in high purity metals. The conventional four-terminal measurement of resistivity becomes difficult with large or irregular specimens or with increasing purity and decreasing temperature. The paper describes an alternative technique, called the eddy current decay method, which greatly reduces the above difficulties. The eddy current measurement process does not require any attachment of leads and, in fact, is totally nondestructive. The eddy current apparatus is described, and some typical applications are presented.

**12586.** De Simone, D. V., **Island in a metric world**, *Panhandle Mag.* **6**, No. 2, 18-22 (Winter 1971-72).

Key words: Business and industry; economy; education; international relations; international standards; international trade; metric; technology assessment.

The article is an adaptation of the report, "A Metric America," which evaluates and distills the findings of the U.S. Metric Study in which thousands of individuals, firms and organized groups, representative of our society, participated. On the basis of all the evidence marshalled in the Study, the report concludes that the United States should change to the metric system through a coordinated national program.

**12587.** Dillon, T. A., Godfrey, J. T., **Pressure broadening of the O<sub>2</sub> microwave spectrum**, *Phys. Rev. A* **5**, No. 2, 599-605 (Feb. 1972).

Key words: Classical trajectory; oxygen; pressure broadening; strong collision.

A general expression for the calculation of pressure broadening for vibrational-rotational lines is derived in the strong-collision model. Classical trajectories and a peaking approximation are used to calculate a unitary scattering operator avoiding perturbation expansions, impact-parameter cutoffs, and straight paths. The latter approximations are not expected to be good when short-range potentials dominate the collision interaction. Use of intermolecular-potential parameters determined from thermodynamics and a simple theory of dispersion forces for O<sub>2</sub> calculations gave excellent agreement with experimental data on the magnitude, temperature and quantum-number dependence of the linewidth parameter.

**12588.** Duncan, A. G., Hiza, M. J., **Heat of mixing derived from liquid-vapor equilibrium data: A study of the argon-methane, normal hydrogen-neon, and normal deuterium-neon systems**, *Ind. Eng. Chem. Fundam.* **11**, No. 1, 38-45 (Feb. 1972).

Key words: Argon-methane; binary liquid mixtures; excess Gibbs free energy; excess thermodynamic properties; heat of mixing; liquid-vapor equilibrium data; normal deuterium-neon; normal hydrogen-neon.

A study of three binary systems of interest in cryogenics was undertaken to demonstrate that an acceptable estimate of the heat of mixing may be derived from carefully measured equilibrium liquid and vapor phase compositions employing conventional gas analysis techniques. New data for the Ar - CH<sub>4</sub> system are presented from which derived excess Gibbs free energy and heat of mixing values were obtained. These data and derived properties are shown to be in good agreement with comparable data



available in the literature. Excess Gibbs free energy and heat of mixing values were derived from phase equilibrium data available in the literature for the  $n\text{H}_2 - \text{Ne}$  and  $n\text{D}_2 - \text{Ne}$  systems in the region of complete liquid phase miscibility. Both of these systems exhibit azeotrope formation in the region studied. For the  $n\text{H}_2 - \text{Ne}$  system, results obtained from the two different sets of data used also were in good agreement.

- 12589.** Durst, R. A., Staples, B. R., **Tris/Tris-HCl: A standard buffer for use in the physiologic pH range**, *Clin. Chem.* **18**, No. 3, 206-208 (Mar. 1972).

Key words: Clinical pH standard; pH standard; physiologic pH; tris(hydroxymethyl)aminomethane and tris pH buffer.

A buffer solution containing tris(hydroxymethyl)aminomethane (0.01667 molal) and its hydrochloride salt (0.0500 molal) is proposed as a pH standard for the physiologically important pH range of 7.3 to 7.5. Standard pH values were assigned to this reference solution at temperatures from 0° to 50 °C by means of measurements of hydrogen/silver chloride cells without transference. At 37 °C, the pH(S) of this buffer solution is 7.382 with a temperature coefficient of  $-0.026\text{pH}/^\circ\text{C}$ . This new standard is more compatible with biologic fluids than is the previously certified phosphate buffer.

- 12590.** Erez, A., **A proposed light-coupled analog system for electrical measurements**, *Proc. Electro-Optic Systems Design Conf., New York, N.Y., Sept. 14-16, 1971*, pp. 183-188 (Industrial and Scientific Conference Management, Inc., Chicago, Ill., Sept. 1971).

Key words: Electro-optical coupling; high voltage measurements; light emitting diodes; operational amplifiers.

The combination of a light emitting diode (LED) and a light detector has been widely used to get electrical isolation of the measuring system from the main electrical circuit. The accuracy of a LED-detector couple is limited by nonlinearity, temperature coefficient, and aging of the LED, and by variations in optical coupling. Therefore, most linear measuring and transmitting systems use the light beam as a carrier. The signal, converted to light pulse frequency modulation, is not affected by optical conditions.

An analog system is proposed to measure relatively low frequency (60 Hz) current and voltage in high voltage systems which must be completely isolated from the measuring instruments. It employs an LED and light detector in an optical feedback path of an operation amplifier. The light emitted by the LED contains the measured signal superimposed on a fixed intensity beam which is controlled by a reference zener diode. Part of the emitted radiation is collected by a light detector which serves as the linear negative feedback element, thereby forcing the emitted LED radiation to follow the input signal. The remainder of the beam is collected and transmitted to a photomultiplier which measures the ratio between the ac signal and the steady-state reference beam. The accuracy of the system is limited by the zener diode and linearity of the feedback light detector. Special care must be taken to select a light detector and amplifier with small leakage and bias currents. Optimal pairing of the electro-optical components, in order to achieve maximum radiation-detection efficiency, is a gallium-phosphide LED (600 – 800 nm) and a photocathode with extended red range.

The expected accuracy of the systems is 0.1%. The mean current in the LED is 1–2 mA.

- 12591.** Falge, R. L., Jr., Wolcott, N. M., **Cluster specific heats in copper-rich Cu-Ni alloys: The effect of iron**, *J. Low Temp. Phys.* **5**, No. 6, 617-650 (Dec. 1971).

Key words: Alloy; clustering; copper Ni iron; ferromagnetism; interactions; magnetic; specific heat; superparamagnetic particles.

The specific heats of three Cu-Ni and two Cu-Ni-Fe samples have been measured in the range 0.4-6 K at compositions in the range 20-43% Ni and ~ 0.2% Fe. The results are described in terms of a Schottky function from which the number of levels and the cluster concentration are determined for each composition. Addition of iron to the 20%-Ni sample results in ~ 1/2 cluster per Fe atom added. The specific heat increases in a magnetic field (known for one sample), which is compatible with the Schottky-like function description of the anomalous term in the specific heat, but is incompatible with the Einstein function description. Another possible interpretation of the observed specific heat anomalies is given in terms of an intercluster cooperative phenomenon.

- 12592.** Farrar, T. C., Druck, S. J., Shoup, R. R., Becker, E. D., **Temperature-dependent  $^{13}\text{C}$  relaxation studies of small molecules**, *J. Amer. Chem. Soc.* **94**, 699-703 (Feb. 1972).

Key words: Chemical shift anisotropy; dipole-dipole; scalar relaxation; spin-rotation;  $T_1$ ;  $T_2$ ;  $^{13}\text{C}$  relaxation.

$^{13}\text{C}$  spin-lattice relaxation times ( $T_1$ ) are reported for 60% enriched samples of  $\text{CH}_3\text{OH}$ ,  $\text{CH}_3\text{I}$ ,  $\text{CH}_3\text{Br}$ ,  $\text{CHBr}_3$ ,  $\text{CHCl}_3$ ,  $\text{CH}_3^{13}\text{COOH}$ , and  $\text{CS}_2$ , each measured over a wide range of temperatures at 15.1 MHz. Data are also given on the magnetic field dependence of  $T_1(^{13}\text{C})$  in  $\text{CH}_3\text{OH}$ ,  $\text{CH}_3\text{I}$ , and  $\text{CH}_3^{13}\text{COOH}$ . The  $T_1$  results, together with nuclear Overhauser enhancements measured for the foregoing hydrogen-containing molecules, as well as for  $\text{CH}_3^{13}\text{COCH}_3$ ,  $^{13}\text{CH}_3\text{COOCD}_3$ , and  $(\text{CH}_3)_4\text{Si}$ , are interpreted in terms of the probable relaxation mechanisms.

- 12593.** Fatiadi, A. J., **Oxidative cleavage of aromatic azines with periodic acid; MO model for the reaction intermediate**, *Chimia* **26**, No. 2, 70-72 (Feb. 1972).

Key words: Acid; benzalazine; cleavage; complex; molecular; orbital; periodic acid; rules; symmetry.

Cleavage of benzalazine (and other azines) with periodic acid may initially involve, as a single step, the addition of  $\text{IO}_4^-$  (or its hydrate) across the conjugated azine system, to give an iodate I(V) complex; this view is supported from MO symmetry rules.

- 12594.** Fey, L., **New signals from an old timer – WWV**, *Broadcast Eng.* **13**, No. 7, 44-46 (July 1971).

Key words: Clocks; h. f. broadcasts; sunspot cycle; time signals; WWV; WWVH.

Although many other changes have occurred in broadcasting over the years those who tune in to the National Bureau of Standards time broadcast stations WWV or WWVH have come to expect the same familiar time signals year after year. But not much longer. Soon a new broadcast will be heard with more kinds of services than before for a wider variety of time and frequency users.

- 12595.** Franklin, A. D., Spal, R., **A method for the precision comparison of the densities of small specimens**, *Rev. Sci. Instr.* **42**, No. 12, 1827-1833 (Dec. 1971).

Key words: Density measurement; hydrostatic; precision; small specimens.

The density of an unknown is compared to that of a set of several standard specimens (weighing about 40 mg each) with a standard deviation in the ratio of densities from a single determination of  $3 \times 10^{-4}$  or better. The apparatus consists of two immiscible liquids and a float in the upper, supporting the specimen in the lower by a wire that passes through the interface. The wire

provides a buoyant force gradient. From the change in position of the float when the unknown is substituted for the standards, the density of the unknown relative to that of the standards can be calculated. Other contributions to the buoyant force gradient are also present; their variation during the course of the measurement established the precision of the measurement.

**12596.** Freeman, D. H., **Interactive gel networks. I. Treatment of simple complexation and masking phenomena**, *Anal. Chem.* **44**, 117-120 (Jan. 1972).

Key words: Acceptor; chromatography; donor complexation; interactive gels; liquid chromatography.

Chemical interactions provide an unlimited basis for extending the separation capabilities provided by gel chromatography. This paper concerns the theory of simple acceptor:donor complexation equilibria, which are treated as idealized associative processes. Equations are developed to predict and interpret chromatographic measurements involving a diffusible solute and solvent, and the nondiffusible gel functional group. Systems treated include: I. Inert species, II. Simple solute:gel complexation, III. Solute:gel complexation with solvent:gel masking, IV. Solute:gel complexation with solvent:solute masking and, finally, consideration of the effects of solute dimerization and solute difunctionality. The results are directly applicable to the experimentally measured solute distribution coefficient.

**12597.** Furukawa, G. T., **Vapor pressures of natural neon and of the isotopes  $^{20}\text{Ne}$  and  $^{22}\text{Ne}$  from the triple point to the normal boiling point**, *Metrologia* **8**, No. 1, 11-27 (Jan. 1972).

Key words: Boiling point; neon; neon isotopes; neon point; triple point; vapor pressure;  $^{20}\text{Ne}$ ;  $^{22}\text{Ne}$ .

Apparatus design and procedures are described for the determination of the vapor pressures of naturally occurring neon ( $^{nat}\text{Ne}$ ) and the pure isotopes  $^{20}\text{Ne}$  and  $^{22}\text{Ne}$  from their triple points (TP) to their normal boiling points (NBP). The data have been fitted to vapor-pressure equations with root-mean-square deviations of  $\pm 2.5$  to  $\pm 4.7$  N/m<sup>2</sup> ( $\pm 0.019$  to  $\pm 0.035$  mmHg). The TP pressures ( $P$ ) and the TP and NBP temperatures ( $T$ ) were found to be:

	TP		NBP $T, K$
	$P$	$T, K$	
$^{nat}\text{Ne}$	$43332 \pm 13$ N/m <sup>2</sup> ( $325.02 \pm 0.10$ mmHg)	$24.553 \pm 0.001$	$27.096 \pm 0.001$
$^{20}\text{Ne}$	$43326 \pm 13$ N/m <sup>2</sup> ( $324.97 \pm 0.10$ mmHg)	$24.540 \pm 0.001$	$27.084 \pm 0.001$
$^{22}\text{Ne}$	$43654 \pm 13$ N/m <sup>2</sup> ( $327.43 \pm 0.10$ mmHg)	$24.687 \pm 0.001$	$27.211 \pm 0.001$

(The temperatures are in terms of the NBS-1955 provisional temperature scale. The figures after the  $\pm$  symbol indicate estimated uncertainties.) The calculated vapor pressures of the isotopic  $^{nat}\text{Ne}$ , based on Raoult's law of solution and the observed vapor pressures of the pure isotopes, are in agreement within the combined precision of the measurements with the observed values of  $^{nat}\text{Ne}$ .

**12598.** Geltman, S., Hidalgo, M. B., **A high energy approximation: II. Hydrogen atom excitation by electrons**, *J. Phys. B: At. Mol. Phys.* **4**, 1299-1307 (1971).

Key words: Born approximation; charge transfer; Coulomb wave; ground state; high energy; hydrogen; rearrangement process; theoretical proton.

The cross sections for the excitation of the 2s, 2p, and 3s states of hydrogen by electron impact are evaluated at high ener-

gy in a first order approximation in which the interaction between the incident electron and target proton is represented by a Coulomb wave final state in the  $T$  matrix. In the usual Born approximation this interaction has a vanishing contribution because of the orthogonality of the atomic states. The evaluated total cross sections converge to the boron result at high energies, but the differential cross sections at large angles show marked disagreement with the Born approximation and reasonable agreement with experiment. We conclude that for non-forward inelastic scattering the Born approximation does not converge to the correct result in the high energy limit.

**12599.** Haber, S., **The error in numerical integration of analytic functions**, *Quart. Appl. Math.* **XXIX**, No. 3, 411-420 (Oct. 1971).

Key words: Best quadrature; error functionals; minimum-norm formulas; numerical analysis; numerical integration; optimal quadrature; quadrature.

$R$  is a simply-connected region in the complex plane, containing the interval  $(a,b)$  on the real axis;  $B$  is a Hilbert space of functions analytic on  $R$ . If  $n$  is a positive integer, the integral over  $(a,b)$  of any  $f \in B$  may be approximated by linear quadrature formulas  $Q(f) = a_1 f(x_1) + \dots + a_n f(x_n)$ . The minimum, over all choices of the  $a_i$  and  $x_i$ , of the norm of the error functional  $E$  defined by

$$E(f) = \int_a^b f - Q(f)$$

is denoted  $E_n^{MN}$ . It is shown that in the most commonly considered cases, if the closed interval  $[a,b]$  is contained in  $R$ , then  $E_n^{MN} = O(C^{-n})$  as  $n \rightarrow \infty$ , for some  $C > 1$ . In one case—previously studied by H. S. Wilf—in which  $b \in R$ , it is shown that  $E_n^{MN} = O(n^{-1/2})$ . Bounds are also found for some error functionals of Gaussian quadrature formulas.

**12600.** Hillhouse, D. L., **Circuit for impulse testing of gas tube lightning arresters**, *Proc. IEEE Fall Electron. Conf., Chicago, Ill.*, Oct. 18-21, 1971, pp. 240-245 (Oct. 1971).

Key words: Gas tube arresters, impulse testing; impulse test circuit, gas tube arresters; impulse testing, lightning arresters, telephone; lightning arrester, telephone; measurement, impulse, telephone arresters; telephone lightning arrester, impulse testing; test circuit, telephone arrester.

Telephone lines may be protected from lightning-induced surges by gas tube lightning arresters. Typical arresters break down at 250-400 volts dc. Breakdown voltage increases with the rate of rise of the applied voltage, and may be two or three times the dc value at a rate of rise of 10 kilovolts/microsecond (kV/ $\mu$ s). Lightning surges on telephone lines approach this rate of rise.

The circuit described in this paper generates and measures ramps with linear rates of rise from 0.5 to 10 kV/ $\mu$ s, chopped at 500 to 1500 volts. In order to achieve ramp linearity and to minimize oscillations after the chop, stray capacitances and inductances must be made as small as possible. Construction and layout required to achieve this are described in some detail, and typical test oscillograms at 0.5 and 10 kV/ $\mu$ s are presented in corroboration. Measurement accuracy is analyzed, and maximum errors are estimated to be, for breakdown voltage, 3% and 10% at 0.5 and 10 kV/ $\mu$ s, respectively; and for rate of rise, 5% for all ramps. If greater accuracy is required, it can be obtained by correction for divider time constant errors, and by further study of carbon resistor voltage coefficients.

**12601.** Hust, J. G., **Thermal conductivity standard reference materials from 4 to 300 K. I. Armco iron**, (Proc. 9th Conf. Thermal Conductivity, Iowa State University, Ames, Iowa, Oct. 6-8, 1969), Chapter in *Thermal Conductivity*, pp. 217-233 (National Technical Information Service, Springfield, Va., 1970).



**Key words:** Cryogenics; electrical resistivity; iron; Lorenz ratio; Seebeck effect; thermal conductivity; transport properties.

Thermal conductivity, electrical resistivity, Lorenz ratio, and thermopower data are reported for several specimens of Armco iron for temperatures from 4 to 300 K. At low temperatures the electrical resistivity and thermal conductivity vary from specimen to specimen by more than 10%. However, the Lorenz ratios of these specimens differ by less than 2.5%; and the intrinsic resistivities calculated using Matthiessen's rule differ by less than 0.5% of the total resistivities. Thus, Armco iron specimens can be used as standards by measuring the residual resistivities and utilizing the Lorenz ratio reported here.

**12602. Johannesen, R. B., Coyle, T. D., Nuclear magnetic double resonance, *Endeavour* XXXI, No. 112, 10-15 (Jan. 1972).**

**Key words:** Double resonance; nuclear magnetic resonance; review.

Double resonance procedures supplement the more conventional techniques of high-resolution nuclear magnetic resonance spectroscopy. Applications of this method allow simplification of complex spectra and facilitate spectrum interpretation and assignment of chemical structures. The technique also permits indirect observation of resonance signals from a wide variety of nuclei.

**12603. Joiner, B. L., Rosenblatt, J. R., Some properties of the range in samples from Tukey's symmetric lambda distributions, *J. Amer. Statist. Ass.* 66, No. 334, 394-399 (June 1971).**

**Key words:** Approximations; distributions, non-normal; lambda distributions; logistic distribution; order statistics; range; statistics; tables; Tukey's lambda distributions.

Tukey introduced a family of random variables defined by the transformation  $Z = [U^\lambda - (1-U)^\lambda]/\lambda$ , where  $U$  is uniformly distributed on  $[0,1]$ . Some of its properties are described with emphasis on properties of the sample range. The rectangular and logistic distributions are members of this family and distributions corresponding to certain values of  $\lambda$  give useful approximations to the normal and  $t$  distributions. Closed form expressions are given for the expectation and coefficient of variation of the range and numerical values are computed for  $n = 2(1)6(2)12, 15, 20$  for several values of  $\lambda$ . It is observed that Plackett's upper bound on the expectation of the range for samples of size  $n$  is attained for a lambda distribution with  $\lambda = n - 1$ .

**12604. Kamper, R. A., Superconducting materials, Chapter 6 in *Electronics Design Materials*, pp. 71-79 (The Macmillan Press Ltd., United Kingdom, 1971).**

**Key words:** Electronics; low temperature; materials; superconductors.

This is a brief survey of the properties of superconducting materials which are of interest for engineering purposes.

**12605. Kamper, R. A., Siegwarth, J. D., Radebaugh, R., Zimmerman, J. E., Observation of noise temperature in the millikelvin range, *Proc. IEEE Lett.* 59, No. 9, 1368-1369 (Sept. 1971).**

**Key words:** Amplifier noise; Josephson effect; low temperature; noise temperature; superconductors.

We report some measurements of noise at very low temperatures, with emphasis on the design and performance of the system used. This system is based on the Josephson effect, and has an observed noise temperature less than 0.005 K.

**12606. Kaufman, V., Minnhagen, L., Accurate ground-term combinations in Ne I, *J. Opt. Soc. Amer.* 62, No. 1, 92-95 (Jan. 1972).**

**Key words:** Neon; spectra; ultraviolet; wavelengths.

The Ne I resonance line  $\lambda 743$  has been accurately measured in the fifth order of the NBS 10.7-m vacuum spectrograph against Ar II Ritz standards in the same order; the measured wavelength is  $743.7195 \pm 0.0002$  Å. This gives for the lowest excited level,  $2p^5(^2P_{1/2})3s[1\ 1/2]_2^\circ$  ( $1s_5$  in Paschen's notation), the value  $134,041.84 \pm 0.04$  cm<sup>-1</sup> relative to the ground level. This result was used to calculate all of the observed  $2p^5nl$  levels relative to the ground level, by use of Ne I observations published during the last two decades and the dispersion formula for air adopted after the publication of *Atomic Energy Levels* (NBS 1949). The  $2p^5\ ^2P_{1/2}^\circ$  ionization energy is  $173,929.75 \pm 0.06$  cm<sup>-1</sup>. From the level system, 46 lines in the vacuum ultraviolet (vuv) between 743 and 576 Å have been calculated according to the combination principle; these should be accurate to  $\pm 0.0002$  Å or better between 743 and 580 Å and to about  $\pm 0.0003$  Å for the few lines below 580 Å.

**12607. Kirchhoff, W. H., On the calculation and interpretation of centrifugal distortion constants: A statistical basis for model testing: The calculation of the force field, *J. Mol. Spectrosc.* 41, No. 2, 333-380 (Feb. 1972).**

**Key words:** Centrifugal distortion; error evaluation; force fields; least squares analysis; model testing; symmetric triatomic molecules.

Watson's treatment of the theory of centrifugal distortion effects is reviewed in detail and special attention is drawn to the relationship between Watson's treatment and the Kivelson-Wilson treatment. The relationship between the distortion parameters and the force field for XYZ-type molecules is also reviewed in order to remove ambiguities and inconsistencies presently found in the literature. Finally, procedures for exploiting the statistics associated with a least-squares analysis of the data are presented as a guide for model testing and for detecting misassignments and mismeasurements. A series of examples illustrating the results of these procedures are presented using the published spectra of SO<sub>2</sub>, OF<sub>2</sub>, SiF<sub>2</sub> and NSF. In the cases of OF<sub>2</sub>, SiF<sub>2</sub> and NSF, improved values for the rotational constants are obtained.

**12608. Kropschot, R. H., Advances in thermal insulation, (Proc. 1970 Cryogenic Engineering Conf., June 17-19, 1970, Colorado Univ., Boulder, Colo.), Chapter in *Advances in Cryogenic Engineering* 16, Paper No. D-1, 104-108 (Plenum Press, Inc., New York, N.Y., 1971).**

**Key words:** Cryogenics; thermal insulation.

This paper highlights several recent developments in insulation which have significant impact upon the cryogenic industry. It emphasizes the gaps in existing data. Complete steady state and transient data are needed over a wide range of temperatures to aid in confirming (or refuting) existing theories. Standard apparatus and standard samples are needed to evaluate the relative merits of competitive insulation schemes.

**12609. Ledbetter, H. M., Patrician, T. J., On the trace analysis of planar features in electron microscopy, *Phys. Status Solidi* 6, No. 1, 305-310 (July 1971).**

**Key words:** Electron diffraction crystallography; twinning.

The effect due to a deviation of the foil plane from the image plane on the trace analysis of planar features in electron microscopy is considered. Analytical expressions are derived for predicting the effects of a known deviation and, conversely, for calculating for some cases the deviation from the observables. Conditions under which the deviation is extreme (maximal or minimal) are enumerated.

**12610.** McDaniel, C. L., Schneider, S. J., **Phase relations in the CaO-IrO<sub>2</sub>-Ir system in air**, *J. Solid State Chem.* **4**, 275-280 (1972).

Key words: CaO:IrO<sub>2</sub> compounds; CaO-IrO<sub>2</sub>-Ir system; dissociation; equilibrium; phase relations.

The equilibrium phase relations for the CaO-IrO<sub>2</sub>-Ir system were determined in air using the quenching technique. The system contains three stable compounds 4CaO·IrO<sub>2</sub>, 2CaO·IrO<sub>2</sub>, and CaO·IrO<sub>2</sub>; they dissociate to an oxide phase, Ir metal, and oxygen at 1240, 1170, and 1135 °C, respectively. A metastable form of CaO·IrO<sub>2</sub> occurs at temperatures between 900 and 1100 °C. Indexed x-ray diffraction powder patterns of all compounds are given.

**12611.** McDonald, D. G., Risley, A. S., Cupp, J. D., Evenson, K. M., **Harmonic mixing of microwave and far-infrared laser radiation using a Josephson junction**, *Appl. Phys. Lett.* **18**, No. 4, 162-164 (Feb. 15, 1971).

Key words: Cryotemperatures; frequency measurements; harmonic mixing; infrared; Josephson junction; superconductivity.

Simultaneous irradiation of a Josephson junction with  $\approx 10$  GHz microwave power and 891-GHz laser radiation produces a 60-MHz beat between the fundamental laser frequency and harmonics of the klystron, ranging from the 84th to the 100th as the klystron is tuned. Observation of such high-order harmonic mixing of klystron and laser signals is unprecedented.

**12612.** Merris, R., **Trace functions I**, *Duke Math. J.* **38**, No. 3, 527-530 (Sept. 1971).

Key words: Character; group; positive semidefinite hermitian matrix; trace.

This paper introduces a natural generalization of the trace of a matrix. The generalization inherits many of the properties of trace and may be substituted for the word "trace" in many theorems, an example of which is: Let  $H$  be a  $pn \times pn$  positive semidefinite hermitian matrix. Partition  $H$  into  $p^2 n \times n$  matrices  $H_{st}$ . Let  $\tau_{st} = \text{tr}(H_{st})$ ,  $s, t = 1, \dots, p$ , and let  $T$  be the  $p$ -square matrix  $T = (\tau_{st})$ . Then  $T$  is positive semidefinite hermitian.

**12613.** Moore-Sitterly, C., **Fundamental spectroscopic data**, *Vistas Astron.* **13**, 161-163 (Mar. 1972).

Key words: Atomic spectra; fundamental spectroscopic data; spectroscopic data.

The primary function of Commission 14 of the International Astronomical Union is to serve in a liaison capacity, i.e. to ascertain the many astrophysical needs in spectroscopy and to survey active laboratory programs with the idea of obtaining the required data. Some aspects of present activity and future needs, as voiced by the Commission, are briefly reviewed here.

**12614.** Newell, A. C., Kern, D. M., **Determination of both polarisation and power gain of antennas by a generalised 3-antenna measurement method**, *Electronics Letters* **7**, No. 3, 68-70 (Jan. 4, 1971).

Key words: Antenna polarisation and gain measurement; extrapolation of near-zone antenna measurements; microwave antenna measurement; near-zone antenna measurement.

A method enabling determination of polarisation and power gain of three unknown antennas, requiring no prior quantitative knowledge of polarisation, is developed. An application of the method using a new near-zone extrapolation technique (introduced by Wacker and Bowman), which permits accurate an-

tenna measurements at reduced distances in spite of proximity effects, is described.

**12615.** Olien, N. A., **The Cryogenic Data Center, an information service in the field of cryogenics**, *Cryogenics* **11**, No. 1, 11-18 (Feb. 1971).

Key words: Critical data; cryogenics; current awareness service; data compilation; information storage and retrieval; information systems; literature searches; National Bureau of Standards.

The Cryogenic Data Center compiles and critically evaluates data on the thermodynamic and transport properties of materials at cryogenic temperatures. The Center also operates an automated information storage and retrieval system covering the field of cryogenics. The paper describes the historical background of the Center and gives a description of the operation of the automated system. There is a brief sketch of the rigorous procedures used in compiling and critically evaluating data. The Data Center has several services which it provides for the general public as well as the staff of the National Bureau of Standards. These services include: a Current Awareness Weekly, quarterly publications on Superconducting Devices and on Liquefied Natural Gas, and conducting literature searches. The Cryogenic Data Center is cooperating with a number of National and International groups in both the data compilation and documentation areas.

**12616.** Olien, N. A., Sarkes, L. A., **LNG-2, A report on the Second International Conference on Liquefied Natural Gas**, *Amer. Gas Ass. Monthly* **53**, No. 2, 12-14 (Feb. 1971).

Key words: Cryogenics; economic forecasts; international conferences; liquefied natural gas; world trade.

The Second International Conference was held in Paris, October 19-23, 1970. More than 1200 persons attended the conference and fifty-five technical papers were presented. The conference was divided into seven technical sessions which covered the following topics: historical background of LNG; future role of natural gas as an energy source; liquefaction cycles; safety and testing; properties of LNG and methane; large-scale storage vessels; sea-going tanker construction and classification; LNG pipelines; importation of LNG from the developing to the developed nations; peak load shaving with LNG, liquefied natural gas as a fuel for aircraft and automobiles; projections on the future growth of world trade involving LNG. The future of liquefied natural gas lies in its use in peak shaving and in importation as base load. The major areas for importation will be Japan and the United States Eastern Seaboard. This trade will increase to about 8 to 10 billion cfd by 1980. Applications of LNG such as an automotive fuel are difficult to predict, because of the dominance of non-qualitative factors such as public opinion in any calculations. The future of liquefied natural gas looks very bright.

**12617.** Peterson, R. L., Magnusson, B., Weissglas, P., **Magnetophonon resonances in polar semiconductors**, *Phys. Status Solidi* **46**, 729-734 (Apr. 14, 1971).

Key words: Acoustoelectric gain; hot electrons; indium antimonide; magnetoresistance; semiconductors; transport theory.

The first numerical calculations are reported of electrical transport properties in polar semiconductors in the non-ohmic regime, for large to intermediate magnetic fields parallel to an electric field. Magnetophonon resonances in such properties as magnetoresistance and acoustoelectric gain are demonstrated. The results obtained generally confirm the hot electron interpretation by Dolat and Bray of their magnetoacoustoelectric experiments in n-InSb.



**12618.** Powell, R. L., Sparks, L. L., **Cryogenic thermocouple research**, (Proc. 11th Intern. Conf. Low Temperature Physics, University of St. Andrews, Scotland, 1968), *Instr. Soc. Amer.* **1**, 477-480 (1968).

Key words: Cryogenics; gold alloys; standard reference data; thermocouples.

Experimental tests and calibrations between 4 and 280 K have been completed for the following materials: Chromel, copper, "normal" silver, constantan, AlumeI and gold-0.07 at.% iron. Many thermocouple combinations can be made from these materials; however, three of the possible pairs are very widely used in the cryogenic temperature range. These are copper vs constantan (type T), Chromel vs AlumeI (type K) and Chromel vs constantan (type E). Our tables for types T, E and K are proposed to be the national standard reference tables for these materials. A fourth combination which is receiving increasing use is Chromel vs gold-0.07 at.% iron. This thermocouple is particularly important because of its relatively high sensitivity even below the normal boiling point of liquid helium. Graphs of voltage and thermopower are presented for this combination. A brief description of the experimental system used in the calibrations will be given. Special methods of data acquisition and analysis have been used to study and minimize systematic errors. These methods are general, but are described as they apply to our particular system.

**12619.** Prydz, R., Straty, G. C., Timmerhaus, K. D., **Calculation of thermofunctions of fluorine**, (Proc. 1970 Cryogenic Engineering Conf., June 17-19, 1970, Colorado Univ., Boulder, Colo.), Chapter in *Advances in Cryogenic Engineering* **16**, Paper No. C-2, 64-77 (Plenum Press, Inc., New York, N.Y., 1971).

Key words: Fluorine; heats of vaporization; saturation; single-phase; thermodynamic properties.

Use is made of newly available *PVT* and specific heat data to calculate thermodynamic functions of gaseous and liquid fluorine to pressures of 21 MN/m<sup>2</sup> (1 MN/m<sup>2</sup> = 10<sup>6</sup> newton/m<sup>2</sup> = 9.86923 atm) and temperatures to 300 K. The calculational procedures are described in detail. Ideal gas properties, which constitute the starting point for the calculations, have been recomputed based on the latest available data. Derived thermo-functions, heat of vaporization and sound velocities, for the single and two phase regions are tabulated.

**12620.** Ruegg, F. W., Shafer, M. R., **Flow measurement: Procedures and facilities at National Bureau of Standards**, (Proc. Symp. Flow Measurement, San Francisco, Calif., Jan. 19-22, 1970), Chapter in *ASHRAE (Amer. Soc. Heat Refrig. Air-Cond. Eng.), Bull. Flow Measurement Part 1*, SF70-7, 1-8 (1972).

Key words: Calibration; flow measurement; flowmeters; flowrate; fluid flow; fluid meters; NBS flow capabilities.

General requirements of flowmeter calibration systems for both liquid and gaseous flow are considered. Possible sources of error are reviewed including those introduced by dynamic characteristics of certain portions of the calibration system. Flowmeter calibration systems in use by the Fluid Meters Section are described including the measurement techniques, operating ranges, and uncertainties associated with these systems.

**12621.** Siegwarth, J. D., Sullivan, D. B., **A mechanical superconducting switch for low temperature instrumentation**, *Rev. Sci. Instr.* **43**, No. 1, 153-154 (Jan. 1972).

Key words: Instrumentation; superconductivity switch.

This paper describes a reliable mechanical superconducting switch for a low temperature voltage divider.

**12622.** Sindt, C., **A summary of the characterization study of slush hydrogen**, *Cryogenics* **10**, No. 5, 372-380 (Oct. 1970).

Key words: Cryogenic pump; densitometer; liquid-solid mixtures; rocket propellant; slurry flow; slush hydrogen.

A programme to study the characteristics of slush hydrogen preparation, storage, transfer, and instrumentation is continuing at the Cryogenics Division of the National Bureau of Standards. Slush preparation by intermittent vacuum pumping was developed. Slush was aged 100 hours during which time solid particle size and structure were observed. The solid particle structure changes dramatically during aging, even though the particle size changes insignificantly. Slush with over 0.5 solid content can be transferred and pumped with losses similar to losses in triple-point liquid hydrogen if Reynolds numbers are high. Transfer losses in a smooth pipe were 10% less with slush of 0.3 solid content than with triple-point liquid when the Reynolds number was  $7 \times 10^5$  or greater. Slush density and mass flow instrumentation are being investigated. Although some special techniques are required for handling slush hydrogen, it has the characteristics of a simple cryogenic fluid for most applications.

**12623.** Sparks, L. L., Powell, R. L., **Laboratory method for assessing homogeneity and interchangeability of thermocouple wires**, *Mater. Res. Std.* **11**, No. 8, 19-21 and 52 (Aug. 1971).

Key words: Cryogenics; dipping; evaluation; heterogeneity; liquid helium; liquid nitrogen; low temperature tests; Seebeck effect; temperature measurement; thermocouples; thermoelectric properties.

Chemical and physical imperfections in thermocouple wire cause spurious voltages to be generated whenever these imperfections are exposed to temperature gradients. For thermometry it is important to know the range of thermally generated spurious voltages to be expected from a specific material. Significant variations usually exist in the thermoelectric properties of widely separated lengths of wire from the same spool or from different melts or from different manufacturers. Simple laboratory methods are described for determining the effect of short range inhomogeneities or inter and intracompany variations. Application of the results obtained from these simple tests is discussed in order to point out the usefulness and limitations of the methods.

**12624.** Straty, G. C., Younglove, B. A., **A fluorine compatible low temperature electrical feedthrough**, *Rev. Sci. Instr.* **43**, No. 1, 156-7 (Jan. 1972).

Key words: Electrical feedthrough; fluorine compatibility; fluorine seal; seal.

A simple seal is described which has been used successfully to seal electrical leads into a cell containing liquid or gaseous fluorine.

**12625.** Sullivan, D. B., Zimmerman, J. E., **Mechanical analogs of time dependent Josephson phenomena**, *Amer. J. Phys.* **39**, No. 12, 1504-1517 (Dec. 1971).

Key words: Josephson effect; mechanical analogy; superconducting devices.

The pendulum analog of a small area Josephson junction is coupled to the analogs of other circuit elements to demonstrate a variety of time dependent phenomena observed with actual devices. The analogy between electrical circuit and mechanical device is established through a Lagrangian formalism. The

analog provides a simple and quick means of developing physical insight into this highly nonlinear system. To demonstrate the value of the analog we consider, as one example, the problem of a junction coupled to a resonant cavity and present a result which was missed by a previous solution.

**12626.** Weisman, H. M., **Technical librarians and the National Standard Reference Data System**, *Special Libraries* 63, No. 2, 69-76 (Feb. 1972).

Key words: Properties data; National Standard Reference Data System; scientific and technical librarians; Special Libraries Association; survey; users.

Because technical librarians often serve as intermediaries between National Standard Reference Data System publications and their users, the Office of Standard Reference Data surveyed by mail 2,700 selected members of the Special Libraries Association to check their knowledge and use of NSRDS publications as well as to learn the problems they encounter in providing the publications or their data to their users. On the basis of a 22% response, the survey results showed that almost 88% of the responders have heard of the NSRDS and that about 59% have indicated that their libraries carry NSRDS publications, but less than 44% of the responders have used an NSRDS publication; however, 94% of this latter percentage (the users) indicated that they have found NSRDS publications very or to some extent useful. The survey revealed that distribution and dissemination procedures of NSRDS publications need improvement and that better ways need to be found to acquaint both librarians and users with the data and information contained in NSRDS publications.

**12627.** Weiss, B-Z, Meyerson, M. R., **Plastic zone formation and fatigue crack extension during high cyclic bending of steels**, *Eng. Fract. Mech.* 3, 475-491 (1971).

Key words: Fatigue crack propagation; fatigue of steels; high cyclic bending; plastic zone sizes; stress intensity factor.

In repeated high cyclic bending, with constant load amplitude, the size and the shape of the plastic zone preceding the propagating crack is controlled by local structural conditions near the tip rather than by stress intensity. No significant correlations were found between the experimentally determined sizes of plastic zone and the theoretically predicted values of Liu and Rice. The plastic zone sizes ahead of the propagating crack cannot be simply expressed as proportional to the rate of fatigue crack propagation, though a simple relationship exists between the rate and the stress intensity factor. The relationship given by Paris,  $dl/dN = Q\Delta K^x$ , describes the rate of crack propagation only in a limited range of relative crack length,  $x < 0.5$ . The extent of this range depends on the structure and on the level of applied cyclic stress. Beyond this range, the Paris equation could not be applied and the crack propagation cannot be related to the stress intensity factor.

**12628.** Abramowitz, S., Acquista, N., **The infrared spectrum of matrix isolated  $\text{UO}_2(\text{g})$  and its thermodynamic properties**, *J. Phys. Chem.* 76, No. 5, 648-649 (1972).

Key words: Entropy; infrared spectrum; matrix isolation; thermal functions;  $\text{UO}_2$ .

The far-infrared spectrum of  $\text{U}^{16}\text{O}_2$  and  $\text{U}^{18}\text{O}_2$  has been observed and assigned. A value of the missing stretching fundamental has been estimated. These vibrational frequencies have been utilized to estimate the  $S^\circ_{2000}$  for reasonable molecular models. A value of  $S^\circ_{2000}$  of  $93.9 \pm 2.0$  eu is estimated for  $\text{UO}_2(\text{g})$  to the harmonic oscillator rigid rotor approximation. Any electronic contributions to the  $S^\circ_{2000}$  have been neglected and a singlet ground state has been assumed.

**12629.** Arenhovel, H., Danos, M., Williams, H. T., **Baryon resonances in nuclei with applications to the two-nucleon system**, *Nucl. Phys. A* 162, 12-34 (1971).

Key words: Baryon resonances; exchange currents; high momentum components; nuclear functions; nuclear magnetic moments; nuclear structure; nuclear wave functions.

The non-relativistic description of the nucleus is presented which allows the possibility of excited baryon resonances within the nucleus via collision of the nucleons with exchanged mesons. A perturbative treatment for the intrinsically excited configurations is justified, and lowest order results for the wave functions of the excited configurations are derived. Detailed formulae for the two-nucleon system are presented and numerical results are given to show the effect of the baryon resonances on the magnetic moment and threshold photodisintegration of the deuteron.

**12630.** Berger, M. J., **Distribution of absorbed dose around point sources of electrons and beta particles in water and other media**, *J. Nucl. Med.* 9, MIRD Supplement No. 5, 6-23 (Mar. 1971).

Key words: Absorbed dose; beta-rays; electrons; internal dosimetry; tissue; water.

This pamphlet presents information about the distribution of absorbed dose around point-isotropic sources of electrons and beta particles. Tabular results are presented for monoenergetic sources with energies between 10 MeV and 25 keV, and for 75 radionuclide beta-ray sources. The data are given for a water medium. Information and procedures are also given by which the data can be adapted to other media of low atomic number, such as tissue, air or plastics.

**12631.** Berger, M. J., **Energy deposition by low-energy electrons: Delta-ray effects in track structure, and microdosimetric event-size spectra**, *Proc. 3d Symp. Microdosimetry, Stresa, Italy, Oct. 18-22, 1971*, EUR No. 4810 d-f-e, pp. 157-177 (1972).

Key words: Delta-ray; electron; energy deposition; event-size spectra; microdosimetric; stopping power; track structure.

The slowing down, diffusion and penetration of low-energy electrons has been calculated by the Monte Carlo method, in order to obtain data of radiobiological interest in two areas. One calculation deals with the energy deposited by the delta-rays around the tracks of heavy charged particles. Absorbed-dose distributions with respect to distance from the primary track axis have been obtained for six initial electron energies (20, 10, 5, 2, 1 and 0.5 keV) and for ten emission angles with respect to the primary track ( $0^\circ, 10^\circ, \dots, 90^\circ$ ). These data have been put in such a form that interpolation with respect to initial delta-ray energy and emission angle is easy. They can be used together with experimental or theoretical information about delta-ray production to study track structure for any heavy charged particle. The second problem is to determine microdosimetric event-size spectra in a medium containing a uniform concentration of the beta-emitter tritium. Comparisons are made with experimental results of Ellett and Braby for spherical sites, with diameters of 1.85 and 0.44 microns, in a propane medium.

**12632.** Blair, B. E., **Letter in response to comments by R. O. Whitaker about the paper, Long-Term Continental U.S. Timing System Via Television Networks**, *IEEE Spectrum* 8, No. 10, 13 (Oct. 1971).

Key words: Clocks; NBS TV timing; time system; TV time dissemination; TV timing system.

A responding communication to a published letter by R. O. Whitaker in *IEEE Spectrum* (Sept. 1971) concerning the published paper, "Long-Term Continental U.S. Timing System



Via Television Networks." (Spectrum-August 1971). We note that a real time system could be available to the general public via television networks. We imply that TV sets could be built with clocks capable of day to day time errors of less than 100 ms.

- 12633.** Bloss, R. L., **An extensometer for use as a laboratory standard at temperatures to 1500 °C**, *ISA Trans.* **10**, No. 3, 242-249 (1971).

**Key words:** Extensometer; high temperature; laboratory standard; strain gage; transient temperature.

Accurate measurement of strain is important in determining mechanical properties of materials and structures and in verifying the capability of structures to meet service conditions. When service conditions include hostile environments, such as high and rapidly changing temperatures, knowledge of the effect of these conditions on the strain gages being used is essential.

An extensometer was developed for use as a laboratory standard for evaluating the performance of remote reading strain gages at high (up to 1500 °C) and rapidly changing (up to 55 °C/s) temperatures. This instrument has a range of more than 2.2 mm, a resolution of  $2.5 \times 10^{-7}$  m, nonlinearity of less than 0.2 percent of range, and random errors of about  $5 \times 10^{-7}$  m. The effect of intense thermal radiation was small. The design, evaluation, and performance of this type of extensometer is discussed.

- 12634.** Borie, E., Maximon, L. C., Olsen, H., **Molecular coherence effects in radiation processes: Bremsstrahlung**, *Phys. Rev. A* **2**, No. 4, 1443-1449 (Oct. 1970).

**Key words:** Bremsstrahlung; electron; interference; molecular coherence; photon spectrum; radiation.

The influence of molecular structure on the bremsstrahlung process at low energies has been studied for diatomic molecules. Interference effects give rise to an increase in the total radiation cross section which is large low electron energies. Although the various cross sections are calculated in Born approximation, the results are expected to be qualitatively correct.

- 12635.** Bowen, R. L., Cleek, G. W., **A new series of x-ray-opaque reinforcing fillers for composite materials**, *J. Dental Res.* **51**, No. 1, 177-182 (Jan.-Feb. 1972).

**Key words:** "Aluminoborate anomaly"; barium; composites; dental materials; glasses; radiopaque; reinforcements.

Clear, colorless glasses that absorb roentgen rays were prepared by melting together compounds yielding silica, barium oxide, boric oxide, and alumina. Barium oxide made the glasses radiopaque and gave the desired refractive index. Boric oxide lowered the melt viscosity, and alumina tended to stabilize the glasses. Some of these glasses seem to be suitable for use as the reinforcing fillers for composite dental restorative materials.

- 12636.** Brady, E. L., Branscomb, L. M., **Information for a changing society**, *Science* **175**, 961-966 (Mar. 3, 1972).

**Key words:** Information packages; information policy; information systems; information users; OECD; technical information.

For society's needs, technical information must be credible, interpreted for various user groups, and repackaged together with other kinds of information in order to be used effectively by decision-makers. Starting from these premises, an Advisory Committee appointed by the OECD Secretary General developed 13 conclusions and recommendations for action by the Organization for Economic Development and its Member States. This paper summarizes the conclusions and recommendations and suggests ways in which the recommendations might be applied in practice.

- 12637.** Branscomb, L. M., **Why people fear technology**, *The Futurist*, p. 232 (Dec. 1971).

**Key words:** Performance standards; pollution; technology.

Many people are "up tight" about technology, due mainly to rising expectations outstripping technology's ability to satisfy them. Six reasons are given for the current anxiety and frustrations the public has toward science and technology.

- 12638.** Brauer, G. M., Termini, D. J., **Bonding of bovine enamel to restorative resin: Effect of pretreatment of enamel**, *J. Dent. Res.* **51**, No. 1, 151-160 (Jan.-Feb. 1972).

**Key words:** Adhesion to bovine enamel; bonding enamel to restorative resins; effect of enamel surface treatment; enamel etch; restorative resins; tensile adhesion.

The efficiency of simple treatments of the enamel surface with various polyfunctional acids and chelating agents was studied to obtain adequate adhesion between tooth surfaces and commercially available acrylic resins. Many water soluble acids induced bonding to enamel. Two ten-second treatments at three minute intervals with acid solutions such as 20% lactic acid may be useful in the clinical treatment of precarious lesions.

- 12639.** Carter, J. C., Coyne, J. J.,  **$SU(6)$  Clebsch-Gordan coefficients for the product  $35 \times 70$** , *J. Math. Phys.* **10**, No. 7, 1204-1210 (July 1969).

**Key words:** Coupling coefficients; permutation symmetry; quark interchange; relative phases,  $SU(6)$  multiplets;  $35 \times 70$ .

A method is presented which makes explicit use of Young diagrams to calculate  $SU(3) \times SU(2)$  multiplet-coupling coefficients in  $SU(6)$ . The multiplet-coupling coefficients for  $35 \times 70$  are given.

- 12640.** Cassinelli, J. P., Hummer, D. G., **Radiative transfer in spherically symmetric systems—II. The non-conservative case and linearly polarized radiation**, *Mon. Notic. Roy. Astron. Soc.* **154**, No. 1, 9-21 (Oct. 1971).

**Key words:** Polarized radiation; radiative transfer; Rayleigh scattering; spherical geometry; stellar atmospheres.

The method for the solution of transfer problems in spherically symmetric systems developed recently by Hummer and Rybicki is here generalized to the non-conservative case. This procedure, which depends on the iterative determination of the Eddington factor  $f = K/J$ , handles in a natural way the outward peaking of the radiation field which occurs in extended atmospheres. To illustrate the present extension of this method, solutions are obtained for the problem of scattering of linearly polarized radiation by an extended electron-scattering atmosphere. Although the transfer of radiation through such an atmosphere is conservative, each of the component equations is not. For opacity laws of the form  $\kappa\rho = r^{-n}$ ,  $0 < r < R$ ,  $n = 2$  and 3, very large values of the polarization are found as a general feature arising from the strong peaking of the radiation field. It is found that the temperature distribution in such extended electron-scattering atmospheres differs negligibly from that computed on the assumption of isotropic scattering, with the neglect of polarization. The procedure used for the polarization problem can also be applied directly to problems with a non-grey opacity involving many frequencies simultaneously.

- 12641.** Coyle, T. D., Ritter, J. J., **Organometallic aspects of diboron chemistry**, Chapter in *Advances in Organometallic Chemistry* **10**, 237-272 (Academic Press, New York, N.Y., 1972).

**Key words:** Boron; boron chemistry; catenated boron compounds; diboron chemistry; organoboron compounds; organometallic chemistry.

This article reviews features of the chemistry of diboron compounds of particular interest from the organometallic viewpoint. Some general features of diboron chemistry are surveyed, with emphasis on unique synthetic aspects and on properties particularly characteristic of compounds containing a simple electron-pair bond between boron atoms. More extensive consideration is given to the interaction of diboron compounds with unsaturated organic systems, which is a major aspect of organometallic chemistry based on boron-boron bonded compounds, and to some of the chemistry of particular organoboron compounds derived from diboron precursors.

**12642.** Danos, M., **Fully consistent phase conventions in angular momentum theory**, *Ann. Phys.* **63**, No. 2, 319-334 (Apr. 1971).

Key words: Angular momentum theory; matrix elements; phase conventions; Racah algebra; recoupling graphs; recoupling transformations.

By a slight modification of the phase conventions of angular momentum algebra, all phases can be eliminated from the formulas. Consequently, a simple, true graphical representation of the complete Racah algebra can be constructed. This way all topological questions of the recoupling transformations can be solved graphically, enabling one to write directly the algebraic expression of the final result.

**12643.** Eisenhart, C., **The assumptions underlying the analysis of variance**, Chapter 7.1 in *Statistical Issues: A Reader for the Behavioral Sciences*, R. E. Kirk, ed., pp. 226-240 (Brooks/Cole Publ. Co., Monterey, Calif., 1972).

Key words: Analysis of variance; chi-square distribution, F-distribution; components of variance; confidence intervals; estimation; fixed effects; Model I; Model II; random effects; tests of significance.

It is shown that familiar partition of "sums of squares" is based on algebraic identities that are valid whatever the interpretation of the numbers involved. Two distinct classes of problems solvable by analysis of variance are recognized: detection and estimation (1) of fixed (constant) relations among the means of sub-sets of the universe of objects concerned; and (2) of components of random variation associated with a composite universe of objects. The corresponding mathematical models are designated *Model I* and *Model II*, respectively. In *Model I* the observations  $X_{ij}$  are normally and independently distributed with a common variance  $\sigma^2$  about (population) mean values  $m_{ij}$  that are conceived to be fixed constants satisfying the additivity relations  $m_{ij} = m_{i.} + (m_i - m_{i.}) + (m_j - m_{.j})$  where the  $m_{i.}$  and  $m_{.j}$  are the corresponding  $i$ th row and  $j$ th column means, respectively, ( $i = 1, 2, \dots, r; j = 1, 2, \dots, c$ ). In *Model II* the same structure is assumed except that the row deviations  $(m_i - m_{i.})$ , ( $i = 1, 2, \dots, r$ ) are no longer conceived to be fixed constants, but normally and independently distributed about zero with common variance  $\sigma_r^2$ ; and the column deviations,  $(m_j - m_{.j})$ , ( $i = 1, 2, \dots, c$ ), normally and independently distributed about zero with common variance  $\sigma_c^2$ . These two models provide necessary and sufficient bases for the two common groups of tests of significance and confidence interval procedures associated with analysis of variance. For purposes of mere unbiased estimation of fixed row and column effects (Model I), or of row and column components of variance (Model II), it is sufficient that the respective random variables  $x_{ij}$  be uncorrelated; the normality assumption is unnecessary except for rigor of the common tests of significance and corresponding confidence interval procedures.

**12644.** Franzen, D. L., Jennings, D. A., **Gain saturation measurements in CO<sub>2</sub>, TEA amplifiers**, *J. Appl. Phys.* **43**, No. 2, 729-730 (Feb. 1972).

Key words: Atmospheric; CO<sub>2</sub>; gain saturation; lasers.

Measurements of gain in CO<sub>2</sub>, TEA pulsed amplifiers operating at a pressure of 330 torr are described. The energy gain in traversing a small amplifying section decreases to one-half the small-signal value at an energy flux density of 1.2 J cm<sup>-2</sup>.

**12645.** Geist, J., **The effect of wall roughness on the spectral density of radiation within symmetric closed cavities in good conductors**, *J. Opt. Soc. Amer.* **62**, No. 4, 602-604 (Apr. 1972).

Key words: Blackbody; electromagnetic radiation; radiometry.

It is shown that roughening the walls of highly symmetric closed cavities in good conductors reduces the deviations of the spectral energy density within the cavity from that predicted by Planck's law. Roughening is most effective at short wavelengths, and it has its most significant effect on de-polarizing the radiation in the cavity.

**12646.** Handy, L. B., Sharp, K. G., Brinckman, F. E., **The metathetical chemistry of halotungsten(VI) compounds. Synthesis and geometry of organooxy fluorides and chlorides**, *Inorg. Chem.* **11**, No. 3, 523-531 (1972).

Key words: Alkoxy; chlorides; exchange reactions; fluorides; methoxy; nuclear magnetic resonance; organosilanes; organoxy; stereochemistry; synthesis; tungsten(VI) halides.

Tungsten(VI) halides can be selectively metathesized with organooxysilanes and, where appropriate, with methoxide ion. Reactions proceed without reduction of the metal and degree of substitution can be regulated by control of stoichiometry. In this manner, the compounds (CH<sub>3</sub>O)<sub>n</sub>WX<sub>6-n</sub>, where  $n = 1 - 4$  and X = F or Cl, can be synthesized from the reaction of CH<sub>3</sub>OSi(CH<sub>3</sub>)<sub>3</sub> and WX<sub>6</sub>. Further substitution does not efficiently take place with CH<sub>3</sub>OSi(CH<sub>3</sub>)<sub>3</sub> but can be effected with CH<sub>3</sub>O<sup>-</sup>, again with maintenance of the W(VI) state, to give the (CH<sub>3</sub>O)<sub>5</sub>WCl and (CH<sub>3</sub>O)<sub>6</sub>W species. The two series may be interconverted via fluorination of W - Cl bonds with SbF<sub>3</sub> or chlorination of W - F bonds with (CH<sub>3</sub>)<sub>3</sub>SiCl. The stereochemical disposition of all products has been determined by <sup>1</sup>H and, where possible, <sup>19</sup>F nmr.

**12647.** Hanson, D. W., Hamilton, W. F., **Clock synchronization from satellite tracking**, *IEEE Trans. Aerosp. Electron. Syst.* **AES-7**, No. 5, 895-899 (Sept. 1971).

Key words: Clocks; propagation delay; satellites; synchronization; time dissemination; tracking.

The tracking of synchronous satellites to provide propagation delays for the synchronization of clocks is described. The tracking is accomplished by range measurements to the satellite from three stations using signals transponded by the satellite. These same signals also functioned as the timing signals for the synchronization of other stations' clocks. Although the range measurements were of low resolution by usual standards, approximately 3000 meters, they provided the delays necessary to synchronize clocks to 40 microseconds or better. These results were obtained over a 4-month period using two satellites with measurements from five stations in the United States and South America.

**12648.** Hubbell, J. H., **Photon cross section compilation activity in the U.S. in the range 1 keV to 100 GeV**, *J. Phys.* **32**, No. 10, C4-14 - C4-20 (Oct. 1971).

Key words: Attention coefficient; compilation; Compton scattering; photo electric effect; photons; x rays.

A brief survey will be presented of photon cross section (attenuation coefficient) measurements available over the range of



photon energies 10 eV to 100 GeV and elements  $Z = 1$  to 100. The results of these measurements, extracted from the 1909-1970 literature, are on file at the NSRDS (National Standard Reference Data Center) (*X-Ray Attenuation Coefficient Information Center*) at the NBS. These data, plus newly-available theoretical values for photoabsorption, scattering and pair-production cross sections, are the subject of continuing evaluation and compilation programs at the NBS, LRL (Lawrence Radiation Laboratory, Livermore) and elsewhere. Present compilation efforts by NBS (10 keV-100 GeV, 23 elements) and by LRL-NBS (1 keV-1 MeV, 87 elements) will be described and compared with input information. Compilation uncertainties from  $Z$ -interpolation and absorption-edge fine-structure will be discussed.

- 12649.** Keller, R. A., Zalewski, E. F., Peterson, N. C., **Enhancement of absorption spectra by dye-laser quenching, II**, *J. Opt. Soc. Amer.* **62**, No. 3, 319-326 (Mar. 1972).

Key words: Absorption; lasers; spectra.

Insertion of samples into a broad-band dye-laser cavity enhances photographic detectability of trace absorptions by approximately three orders of magnitude. Optical densities as small as 0.0004 were readily detected in a dilute solution of  $\text{Eu}(\text{NO}_3)_3$ . In a modified technique the bandwidth of the dye laser was reduced by using prisms, and the wavelength of this narrow band was swept through the absorption. The modified technique permitted detection of optical densities as small as 0.01. Solutions of theoretical equations describing both processes give good agreement with experimental results, and they provide insight into the mechanism of the effect. The measurements with the broad-band laser could be made in 100 ns or less; therefore, this technique should provide a powerful tool for detection of short-lived transients in very small concentrations.

- 12650.** Kraft, R., **Convergence of semidiscrete approximations of linear transport equations**, *J. Math. Anal. Appl.* **37**, No. 2, 412-431 (Feb. 1972).

Key words: A-priori bound; convergence; finite differences; hyperbolic equation; positive mapping; semi-discrete approximations; transport equation.

A technique will be presented for establishing the convergence of semi-discrete methods of approximating linear transport equations. The technique is based on the "positivity" property of the system of hyperbolic equations which approximate the transport equation. A-priori bounds are deduced by using 1) the properties of Riemann functions that are associated with the hyperbolic systems; and 2) the "positivity" of the hyperbolic systems. The a-priori bounds are then used to deduce convergence in the classical way and obtain decay rates.

- 12651.** Kuyatt, C. E., Natali, S., Di Chio, D., **Accurate calculation of properties of the two-tube electrostatic lens. III. Aberration coefficients**, *Rev. Sci. Instr.* **43**, No. 1, 84-87 (Jan. 1972).

Key words: Fifth-order aberration coefficients; intrinsic aberration coefficients; meridional electron trajectories; third-order aberration coefficients; two-tube electrostatic lens.

Using numerical methods, electric fields and meridional electron trajectories have been calculated for the two-tube electrostatic lens with sufficient precision to determine values for all the third-order and several of the fifth-order aberration coefficients for meridional trajectories. The aberration coefficients are expressed in a form which is intrinsic to the lens and do not depend on a particular object and aperture position. Results were obtained for voltage ratios of 2, 5, 10, 20, and 40.

- 12652.** Kuyatt, C. E., Natali, S. V., Di Chio, D., **Third-order aberration coefficients of electron lenses**, (Proc. 11th Symp. Electron, Ion, and Laser Beam Technology, University of Colorado, Boulder, Colo., May 12-14, 1971), Chapter in *Record of 11th Symposium on Electron, Ion, and Laser Beam Technology*, R. F. M. Thornley, ed., pp. 177-181 (San Francisco Press, Inc., San Francisco, Calif., 1971).

Key words: Electron lenses; experiment; theory; third-order aberration.

In the standard treatments of aberration coefficients of electron lenses, deviations from perfect imagery are expressed as power series of the ray coordinates in the object and aperture planes. The resulting aberration coefficients depend on the object and aperture positions, and a complete description of the aberrations of a lens would, in principle, require a doubly infinite set of aberration coefficients.

Verster has formulated the third-order aberrations of electron lenses in an object- and aperture-independent way for meridional trajectories and has determined some of the coefficients. Using highly precise numerical methods, we have calculated electric fields and electron trajectories in the two-tube electrostatic lens for voltage ratios from 1.5 to 50, and have derived all of Verster's third-order aberration coefficients.

- 12653.** LaVilla, R. E., Deslattes, R. D., **Single and multiple vacancy effects in molecular x-ray spectra**, *J. Phys.* **32**, No. 10, C4-160-C4-164 (Oct. 1971).

Key words:  $\text{Cl } K\beta$ ,  $\text{CH}_3\text{Cl}$ ; double electron process;  $L_{23}$  of argon, Cl and K in KCl; molecular x-ray emission; multiple vacancies.

The x-ray  $K\beta$  emission spectra from molecular gases is discussed with the use of a particular example,  $\text{CH}_3\text{Cl}$ . With the help of a crude threshold experiment, the multiple vacancy processes are shown to be on the high energy side of the prominent spectral lines in Cl  $K\beta$  emission from  $\text{CH}_3\text{Cl}$ . From a recent molecular orbital calculation, the Cl  $K\beta$  molecular emission lines are identified as the  $3e$  and  $7a_1$  orbitals of  $\text{CH}_3\text{Cl}$ . The valence  $K$  emission spectra can be interpreted for the most part in terms of one electron single vacancy transitions from inner shells to the various outer molecular orbitals, where the spectral line position and intensity are dependent on the molecular term value, symmetry and orbital overlap. In the course of extending the x-ray molecular emission studies to the  $L$  series of sulphur and chlorine we measured the  $L_{23}$  spectra from argon gas to study the instrumental response in this region. A prominent *extra* low energy emission feature was found in the Ar  $L_{23}$  spectra. A similar feature is also observed in the  $L_{23}$  emission of Cl and K from KCl. These *extra* features are interpreted as evidence of a double electron process.

- 12654.** Levin, I. W., Abramowitz, S., Müller, A., **Jahn-Teller vibrations of  $\text{ReF}_6$** , *J. Mol. Spectrosc.* **41**, No. 2, 415-419 (Feb. 1972).

Key words: Coriolis constant; force fields; hexafluoride; Jahn-Teller;  $\text{ReF}_6$ .

Model force fields are investigated in order to estimate the unpublished frequencies  $\nu_2^*$  and  $\nu_3^*$  of the molecule  $\text{ReF}_6$  which exhibits a dynamic Jahn-Teller effect. The force fields were estimated using the Coriolis constant  $\zeta_3$  observed from the unresolved vibration rotation band contour of  $\nu_3$  and the other observed frequencies  $\nu_1$ ,  $\nu_3$ ,  $\nu_4$ , and  $\nu_5$ .

- 12655.** Lutz, G. J., **Determination of lead in environmental samples by photon activation analysis**, *Proc. Am. Nucl. Soc. Topical Meeting on Nuclear Methods in Environmental Research*, Aug. 23-24, 1971, Columbia, Mo., pp. 144-149 (Aug. 1971).

Key words: Biological samples; environmental samples; lead; photon activation analysis; soil.

Photon activation analysis has been applied to the determination of lead in environmental samples. Electrons are accelerated to a suitable energy (20-45 MeV) with a linear accelerator and allowed to strike a tungsten target. High energy photons, called bremsstrahlung, are produced from the interaction of the electrons with the coulomb field of the tungsten atoms. Part of this bremsstrahlung is of sufficiently high energy to induce the reaction  $^{204}\text{Pb}(\gamma, n)^{203}\text{Pb}$ .  $^{203}\text{Pb}$  has a half-life of 52 hours and decays with the emission of a 279 keV gamma ray.

After irradiation the sample is either counted nondestructively with a Ge(Li) detector or the lead is separated after dissolution of the sample by extraction into methyl isopropyl ketone or by more rigorous methods and then counted with a Ge(Li) or NaI(Tl) detector.

Precision and accuracy have been determined to be adequate by analyzing some soil and biological samples which had been assayed for lead by other methods. Interfering photonuclear reactions do not occur below 45 MeV.

The limit of nondestructive determination with a Ge(Li) detector is about 0.5 ppm. With a rigorous separation, about 10 nanograms can be determined.

**12656.** McCarter, R. J., **The cause of anomalous behavior in the vertical flammability test**, *Text. Chem. Color* **4**, No. 4, 91-93 (Apr. 1972).

Key words: Flammability; strip tests; testing; testing equipment; vertical tests.

Experiments were conducted to determine the cause of anomalous results in vertical flammability testing. Some fabrics of marginal flammability had indicated an increased tendency to support flame propagation when the time of exposure to the test flame was decreased.

The severity of the vertical test procedure was found to be a maximum when the burner was applied for only the interval necessary for ignition of the sample. With a longer application of the burner to fabrics of marginal flammability, the burning of the fabric may be extinguished by the less-than-ambient oxygen content of the burner plume.

**12657.** Mangum, B. W., Lee, J. N., Moos, H. W., **Magnetically controllable cooperative Jahn-Teller distortion in  $\text{TmAsO}_4$** , *Phys. Rev. Lett.* **27**, No. 22, 1517-1520 (Nov. 29, 1971).

Key words: Cooperative distortion; Jahn-Teller distortion; magnetically controllable distortion; rare-earth;  $\text{TmAsO}_4$ .

$\text{TmAsO}_4$  undergoes a cooperative Jahn-Teller distortion at 6.0 K. At  $T < 6$  K there is a temperature-dependent critical field  $\vec{B}_c$  at which a cooperative distortion back to the high-temperature phase occurs. For  $B < B_c$ , the distortion directions in the basal plane are the (110) and the (1 $\bar{1}$ 0) directions and are magnetically controllable.

**12658.** Mavrodineanu, R., **Discussion of some experimental and fundamental conditions in analytical flame spectroscopy**, *Proc. 3d Intern. Conf. Atomic Absorption and Atomic Fluorescence, Paris, France, Sept. 27-Oct. 1, 1971*, pp. 39-60 (1972).

Key words: Flame; hydrogen; long-path burner; multichannel spectrometer; non-metals; overexcitation; phosphorus; spectrometry; sulfur; triple pass on-axis.

A flexible multichannel flame spectrophotometer was designed and built to extend the measuring capabilities of analytical methods in which a combustion flame is used to emit

or absorb specific radiations. This instrument is composed of a 1 meter spectrometer with its multichannel phototube housing, the appropriate electronic components for scanning and ac and dc signal measurement with integration and printout and a punch tape arrangement for computer calculations. A unique feature of the measurement system is an NBS designed burner and sprayer made of pure alumina with a water cooled tantalum flame plate, which provides an unusually stable flame and hence improved precision of measurement. The instrument can be used as a scanning monochromator, a spectrograph, or a multichannel spectrometer, by appropriate arrangement at the focal plane of the spectrometer. The instrument is used for the simultaneous determination of Na, K, Ca and Mg in biological fluids using Li as an internal standard. The instrument provides the full advantages of specificity, sensitivity, speed and economy of sample in simultaneously obtaining data suitable for rapid computer evaluation. The water-chilled hydrogen flame is described and its capability to excite non-metals is illustrated using P and S as examples. The spectra of HPO and  $\text{S}_2$  are presented together with the mechanism suggested for their production.

**12659.** Merris, R., **A dominance theorem for partitioned hermitian matrices**, *Trans. Amer. Math. Soc.* **164**, 341-352 (Feb. 1972).

Key words: Associated transformation; generalized matrix function; (group) character; Hadamard (Schur) product; Kronecker product; orthogonality relations; Schur function.

Let  $A = (A_{ij})$  be a partitioned positive semidefinite hermitian matrix, where  $A_{ij}$  is  $n$ -square,  $1 \leq i, j \leq m$ . A class of ordered pairs of functions  $(f_1, f_2)$  is given such that  $(f_1(A_{ij}) - f_2(A_{ij}))$  is positive semidefinite hermitian. Applications are given.

**12660.** Mielenz, K. D., Eckerle, K. L., **Accuracy of polarization attenuators**, *Appl. Opt.* **11**, No. 3, 594-603 (Mar. 1972).

Key words: Accuracy; phase retardation plates; polarization attenuators; sheet polarizers; spectrophotometry; transmittance standards.

The accuracy of various polarization attenuators is discussed, including systematic errors due to imperfections of the polarizers, setting errors of the rotating elements, alignment errors of fixed elements, and errors caused by oblique incidence and partial polarization of the incident light. Whereas the accuracy of conventional three-polarizer attenuators is limited to 0.001 transmittance unit, at least ten times more accuracy can be achieved with two new types of attenuators, which employ either a half-wave or a quarter-wave retardation plate in conjunction with two sheet polarizers.

**12661.** Mighell, A. D., Reimann, C. W., Santoro, A., **The crystal and molecular structure of dimeric dibromobis(pyridine  $N$ -oxide) copper(II)**,  $[(\text{pyridine } N\text{-oxide})_2\text{CuBr}_2]_2$ , *Acta Cryst.* **B28**, Part 1, 126-134 (Jan. 1972).

Key words: Bromine; copper; crystal; pyridine  $N$ -oxide; structure; x ray.

The crystal and molecular structure of dimeric dibromobis(pyridine  $N$ -oxide) copper(II),  $[(\text{C}_5\text{H}_5\text{NO})_2\text{CuBr}_2]_2$ , was determined by single-crystal x-ray diffraction techniques. This compound crystallizes in the triclinic system with  $a = 10.510$  (2),  $b = 10.883$  (1),  $c = 11.818$  (5) Å,  $\alpha = 78.57$  (3),  $\beta = 89.88$  (3),  $\gamma = 81.17$  (1)°, space group  $P1$ ,  $\rho_0 = 2.08$ ,  $\rho_c = 2.10$  g·cm $^{-3}$  and  $Z = 2$ . The structure was solved by Patterson and electron-density Fourier techniques and refined by block-diagonal least-squares analysis to a final  $R$  value of 0.046 based on 4415 observed reflections. The structure consists of two centrosymmetric dimeric molecules crystallographically nonequivalent. The centers of symmetry of the two molecules are located at the origin and at the center of the unit cell. In both



dimers each copper atom is coordinated by two bromine atoms, and by three oxygen atoms of which two are bridging. The bromine atoms are located above and below the plane defined by the copper atoms and the bridging oxygen atoms. The two dimeric molecules show significant differences in some bond distances and angles and in the relative orientation of the pyridine *N*-oxide molecules. The geometry of this complex differs markedly from that of its chloride analog, as well as from that of other members of the aromatic *N*-oxide copper(II) halide series. The magnetic properties of the bromide complex are discussed in relation to those of related compounds.

**12662.** Miles, B. M., Wiese, W. L., **Critical evaluation of transition probabilities for Ba I and Ba II**, *Atomic Data* **1**, 1-17 (1969).

Key words: Ba I; Ba II; line strengths; oscillator strengths; transition probabilities.

Transition probabilities for allowed lines of Ba I and II, based on a critical evaluation of available literature sources, are presented in order of increasing quantum numbers.

**12663.** Milligan, D. E., Jacox, M. E., **Infrared and ultraviolet spectroscopic studies of a number of small free radicals and molecular ions in a matrix environment**, Chapter 1 in *Advances in High Temperature Chemistry* **4**, 1-24 (Academic Press, Inc., New York, N.Y., 1971).

Key words: Free radicals; infrared spectrum; matrix isolation; molecular ions, photolysis; ultraviolet spectrum.

The development of the matrix isolation technique is summarized, and the principles which have been found to be important for the *in situ* photoproduction of free radicals trapped in inert solid matrices in sufficient concentration for direct infrared and ultraviolet spectroscopic observation are considered. A survey of the small free radical species heretofore studied using these techniques is given. Examples of the successful application of the technique are drawn from recent studies of the vacuum-ultraviolet photolysis of matrix-isolated methane and silane and of their chloro- and fluoro-derivatives. Results of experiments designed to permit the trapping in inert, non-ionic matrices of negatively charged molecular ions are presented.

**12664.** Moore, G. A., **Gestalt properties of aggregate materials**, *Prakt. Metallogr.* **IX**, No. 2, 76-97 (Feb. 1972).

Key words: Analysis of microstructures; automatic image analysis; Gestalt of a material; microarchitecture; patternness; scanning microscopes; television microscopes.

From the viewpoint of materials engineering and quality control the significant aspects of the microstructure of a material as a whole constitute a Gestalt which controls mechanical behavior. Such a Gestalt has in the past often been specified by the thermal-mechanical history of the material. Higher precision and sound scientific practice require that the specification should be in terms of a properly selected set of measurements of the microstructure. The Gestalt of any aggregate material can be adequately specified by six stereologically valid parameters measuring phase concentration ( $V_V$ ), size ( $\bar{I}_\beta$ ) and spacing ( $\bar{I}_\alpha$ ) of particles, variability between portions of the material ( $V.I.$ ), general anisotropy ( $\bar{I}_1/\bar{I}_2/\bar{I}_3$ ), and degree of patternness ( $S.I.$ ). Raster scanning devices of either the mechanical or television type are intrinsically capable of easily measuring these six parameters. Only minor changes are required to provide this common set of measurements from all scanning instruments and to improve accuracy. In contrast, microarchitectural processes which identify, measure, and selectively count individual object sections require massive effort and have limited relation to behavior; thus are to be avoided whenever feasible.

**12665.** Natali, S., Di Chio, D., Uva, E., Kuyatt, C. E., **Accurate calculation of properties of the two-tube electrostatic lens. II. First-order focal properties and *P-Q* curves**, *Rev. Sci. Instr.* **43**, No. 1, 80-83 (Jan. 1972).

Key words: Electric field; first-order focal properties; paraxial electron trajectories; *P-Q* curves; two-tube electrostatic lens.

Using digital methods, electric fields and paraxial electron trajectories in the two-tube electrostatic lens have been calculated, and the first-order (Gaussian) focal properties accurate to at least 0.1% were obtained for voltage ratios from 1.5 to 50. The results are presented in the form of *P-Q* (object-image position) curves for maximum ease of use.

**12666.** Opal, C. B., Peterson, W. K., Beaty, E. C., **Measurements of secondary-electron spectra produced by electron impact ionization of a number of simple gases**, *J. Chem. Phys.* **55**, No. 8, 4100-4106 (Oct. 15, 1971).

Key words: Atmospheric gases; ionization; noble gases; secondary electron collisions.

The energy distribution and angular dependence of secondary electrons generated by the impact of 100-2000-eV electrons on He, N<sub>2</sub>, and O<sub>2</sub> and by the impact of 500-eV electrons on Ne, Ar, Kr, Xe, H<sub>2</sub>, NO, CO, H<sub>2</sub>O, NH<sub>3</sub>, CH<sub>4</sub>, C<sub>2</sub>H<sub>2</sub>, and CO<sub>2</sub> have been measured over the 4-200-eV range. The measurements were made in a crossed-beam apparatus with the use of a fixed hemispherical electrostatic analyzer and a rotatable electron gun. The observed spectra were integrated over angle to obtain relative cross sections for secondary-electron production. It was found that the shapes of the spectra of all the gases (except Ar, Kr, and Xe, which contain intense electron emission features in this energy range) were smooth and qualitatively similar, approaching a constant cross section at low secondary energies, and falling off at high secondary energies slightly faster than  $E_s^{-2}$ , where  $E_s$  was the energy of the secondary. The shape of the spectrum was found to be nearly independent of primary energy in He, O<sub>2</sub>, and N<sub>2</sub>.

**12667.** Ott, W. R., **Measurement of transition probabilities for O I in the vacuum ultraviolet**, *Phys. Rev. A* **4**, No. 1, 245-251 (July 1971).

Key words: Arc emission; oxygen; transition probability; vacuum ultraviolet.

Transition probabilities for O I lines emitted in the vacuum ultraviolet were measured using a wall-stabilized arc discharge operating in a mixture of argon and oxygen. The lines were emitted from a column of plasma which was observed end-on and which was characterized by a nearly uniform temperature. Optically thin conditions were achieved by reducing the relative concentration of oxygen atoms in the discharge to levels of less than one part per million. Absolute values for the O I transition probabilities were obtained by determining the oxygen-atom density and plasma length through a measurement of the absolute intensity of the O I  $\lambda = 7773.4$  Å line, whose transition probability is known. The following values were measured for lines in the resonance transition array:  $A(^1D_2 - ^1D_2, \lambda = 1152 \text{ Å}) = 5.5 \times 10^8 \text{ sec}^{-1}$ ;  $A(^1S_0 - ^1P_1, \lambda = 1218 \text{ Å}) = 1.8 \times 10^8 \text{ sec}^{-1}$ ;  $A(^3P_0 - ^3S_1, \lambda = 1306 \text{ Å}) = 0.66 \times 10^8 \text{ sec}^{-1}$ ;  $A(^3P_{2,1,0} - ^3S_1, \lambda = 1303.5 \text{ Å}) = 5.9 \times 10^8 \text{ sec}^{-1}$ . These values are in excellent agreement with recent lifetime measurements. Existing discrepancies in the literature concerning a previous arc determination of the O I vacuum ultraviolet oscillator strengths by Boldt and Labuhn are discussed. The present method is considered to be an improvement over the method used by Boldt and Labuhn which relied, first of all, upon extrapolation techniques to reach the linear part of the curve of growth and, secondly,

upon a complex calculation of the oxygen-atom number density using basic conservation equations.

- 12668.** Piccirelli, R. A., **Theory of the dynamics of simple fluids for large spatial gradients and long memory**, *Phys. Rev.* **175**, No. 1, 77-98 (Nov. 5, 1968).

**Key words:** Current autocorrelations; noninstantaneous effects; nonlinear effects; nonlocal effects; statistical mechanical theory; transport properties.

A generalization of the classical fluid dynamics which describes noninstantaneous, nonlocal, and nonlinear responses of flows to the thermodynamic forces (gradients) is derived by statistical-mechanical methods. The conservation equations determining the mass, momentum, and energy densities are unchanged in form, but new expressions are given for the pressure tensor and heat current vector. The new expressions are specified functionals of the temperature, flow velocity, and Helmholtz free energy, density, are determined by microscopic quantities (e.g., interparticle potential), and consist of a reversible and an irreversible part. The reversible parts are the expected fluxes in a local-equilibrium ensemble that includes nonlocal effects. The reversible contribution to the heat current is nonvanishing for large enough gradients. The expressions for the irreversible parts are the analog of the classical transport relations, and are linear combinations of integrals over space and time of correlation-function kernels convoluted with the thermodynamic forces. The kernels, which are specified functionals of the fluid densities and are a kind of local-equilibrium correlation of subtracted fluxes, are natural generalizations of the autocorrelation expressions for the classical transport coefficients.

- 12669.** Powell, F. X., Johnson, D. R., **Microwave spectrum of the BrO free radical**, *J. Chem. Phys. Letters to Editor* **50**, No. 10, 4596 (May 15, 1969).

**Key words:** BrO; free radical; magnetic hyperfine; microwave spectrum; rotational spectra; transient species.

The gas phase microwave spectrum of the BrO free radical has been detected in the ground  $^2\Pi_{3/2}$  state. BrO was produced by the reaction of oxygen atoms with molecular bromine at low pressures. Measurements have been made in the hyperfine patterns for the  $J=5/2 \leftarrow 3/2$  rotational transitions of both  $^{79}\text{BrO}$  and  $^{81}\text{BrO}$ . Effective rotational constants, lumped magnetic hyperfine parameters and nuclear quadrupole coupling constants were determined for each isotopic species.

- 12670.** Powell, R. C., **Precision coaxial connectors**, Chapter in *Advances in Microwaves* **6**, 1-28 (Academic Press, Inc., New York, N.Y., 1971).

**Key words:** Coaxial; connectors; microwave; precision measurements; standards.

The evaluation and status of precision coaxial connectors are reviewed. Discussed are: precision coaxial lines, general and laboratory precision connectors, dielectric supports, and coupling mechanisms. Applications are given and an extensive bibliography is included.

- 12671.** Price, D. L., Rowe, J. M., Rush, J. J., Prince, E., Hinks, D. G., Susman, S., **Single crystal neutron diffraction study of potassium cyanide**, *J. Chem. Phys.* **56**, No. 7, 3697-3702 (Apr. 1, 1972).

**Key words:** Cyanide ion; disorder; ion displacements; lattice dynamics; libration; neutron diffraction; potassium cyanide.

Neutron diffraction measurements were made on single crystals of KCN to obtain information about the disorder of the  $\text{CN}^-$  ions in the cubic phase. The crystals were obtained by

pulling from the melt by a modified Czochralski method. Data were collected on two four-circle diffractometers at room temperature and at 180 K, just above the cubic-orthorhombic phase transition. Structure factors were obtained for 24 inequivalent reflections. Free rotation of the  $\text{CN}^-$  ions is ruled out by the different structure factors obtained for reflections with equal values of  $(h^2 + k^2 + l^2)$  but different  $(h, k, l)$ . However, models fitted to the data assuming orientations along a particular symmetry direction did not establish a preferred direction. The fits indicated that both vibrational and librational thermal amplitudes are large and relatively independent of temperature. These amplitudes could not be reproduced by a dynamical model assuming harmonic forces even when rotational-translational coupling was included. A tentative explanation of these results is given in terms of rapid  $\text{CN}^-$  reorientations caused by the low activation energy for rotation.

- 12672.** Prydz, R., **An improved oxygen vapor pressure representation**, *Metrologia* **8**, No. 1, 1-4 (Jan. 1972).

**Key words:** Critical point; oxygen; temperature scales; triple point; vapor pressure equation.

Oxygen vapor pressure measurements reported in the literature have been critically evaluated and the most consistent and reliable of the data sets have been correlated with a vapor pressure equation. However, the data were first adjusted for temperature scale differences to conform with the IPTS-68 temperature scale. "Best" values for the oxygen triple point and critical point parameters were selected for use as indirect constraints in the equation. Pressures obtained from this equation are compared to corresponding values calculated from other published oxygen vapor pressure equations. A new value for the critical pressure of oxygen of  $5.043_2 \text{ MN/m}^2$  (49.77 atm) is given.

- 12673.** Rankin, K., Tauber, S. J., **Linguistics as a basis for analyzing chemical structure diagrams**, *J. Chem. Doc.* **11**, No. 3, 139-141 (1971).

**Key words:** Atom symbols; bond symbols; chemical diagrams; formal grammar; language; linguistic analysis; natural groups; numerical subscripts; patterns; strings; vocabulary.

Chemical structure diagrams constitute a language in the same sense that English and Fortran are languages. A language consists of combinations of members of a vocabulary. For chemical structure diagrams the vocabulary includes atom symbols, bond symbols, and numerical subscripts. In contrast to languages such as English and Fortran, wherein utterances are linear strings, the chemical diagram language uses arrangements of vocabulary members in two dimensions. The linguist seeks to construct a grammar which reflects the chemist's ability to distinguish between valid chemical structure diagrams and other patterns built from the same vocabulary. Such grammar should also account for "natural groups" in valid diagrams.

- 12674.** Reader, J., Ekberg, J. O., **Resonance lines of Ce v and Ce vi**, *J. Opt. Soc. Amer.* **62**, No. 3, 464 (Mar. 1972).

**Key words:** Cerium; spectra.

The spectra of Ce v and vi were photographed with sliding sparks in the vacuum ultraviolet. The five resonance lines of the type  $5p^6 \ ^1S_0 - 5p^5d$  and  $6s, J=1$  for Ce v and the two resonance lines of the type  $5p^5 \ ^2P_{1/2, 3/2} - 5s5p^6 \ ^2S_{1/2}$  are reported here. Identifications of upper levels are based on isoelectronic comparisons.

- 12675.** Reader, J., Epstein, G. L., Ekberg, J. O., **Spectra of Rb II, Sr III, Y IV, Zr V, Nb VI, and Mo VII in the vacuum ultraviolet**, *J. Opt. Soc. Amer.* **62**, No. 2, 273-284 (Feb. 1972).



Key words: Molybdenum; niobium; rubidium; spectra; strontium; ultraviolet; wavelengths; yttrium; zirconium.

The characteristic resonance-line spectrum in the Kr I isoelectronic sequence, consisting of the five transitions to the  $4p^6\ ^1S_0$  ground state from levels with  $J=1$  in the  $4p^54d$  and  $5s$  configurations has been observed from Rb II to Mo VII. The observations were made with sliding sparks, on the 10.6-m normal-incidence spectrograph at NBS and 5-m grazing-incidence spectrograph in Lund. A number of transitions from higher levels of the type  $4p^5nd$ ,  $4p^5ns$ , and  $4s4p^55p$  were also observed. Isoelectronic comparisons are given for all observed levels. The ionization energies in electron volts are

Rb II	27.285	Y IV	60.60	Nb VI	102.06
Sr III	42.87	Zr V	80.36	Mo VII	125.66

Anomalous relative intensities observed for the  $4p^54d$  transitions are found to be caused by excitation conditions within the light source.

- 12676.** Rook, H. L., LaFleur, P. D., Gills, T. E., **Mercury in coal: A new Standard Reference Material**, *Environ. Letters* 2, No. 4, 195-204 (1972).

Key words: Activation analysis; coal; mercury; pollution; standard reference material.

Sources of environmental mercury contamination are generally related to industrial and mining activity. However, close examination of the sources reveal how complex the task of dealing with mercury pollution is. For example, virtually none of the mercury in fossil fuel is trapped in the fly ash, instead it is released in gaseous form as a product of combustion. Evidence now exists that this gaseous mercury is washed from the air by rain, being cycled to rivers, lakes and oceans where further evidence indicates that it may be methylated to its most toxic form, methylmercury.

Mercury releases to the environment from burning of fossil fuels have been calculated to contribute a significant portion of the total mercury released. Unfortunately, mercury concentrations in coals used to calculate mercury release differ by a wide range. This paper presents the results of a concerted analytical program by the National Bureau of Standards to develop a coal standard of proven homogeneity with an accurate value of mercury concentration. This standard was used in determining the mercury level in a suite of coal samples issued by the U.S. Bureau of Mines. The results of this work indicate a range of mercury levels from approximately 0.05 to 0.5 ppm with the average level of 0.1 to 0.2 ppm.

- 12677.** Ruthberg, S., **Standards and vacuum measurements accuracy**, *J. Vacuum Sci. Technol.* 9, No. 1, 186-195 (Jan.-Feb. 1972).

Key words: Absolute vacuum reference standards; dynamic pressure division; manometry; McLeod gage; static pressure division; vacuum measurements accuracy; vacuum standards.

Present capabilities for precision and accuracy are compared with the needs at the working level. A measurements structure is sketched by which reference standards accuracies are propagated. Uncertainties are prescribed for a number of prevalent measurement methods including precision U-tube manometer, McLeod gage, volumetric pressure division, and dynamic expansion. The development at the National Bureau of Standards of direct absolute measurements standards of high precision and their use in dynamic environments stabilized to better than one part in  $10^3$  and ranging from the medium to the ultrahigh vacuum are described. These methods include precision liquid columns for the upper pressure range, interferometer

manometer and modified McLeod gages for the high vacuum range, and a torsion microbalance or vane gage for the ultrahigh vacuum range.

- 12678.** Saylor, C. P., **Case of the flowing roof**, *Chemistry* 44, No. 11, 19-20 (Dec. 1971).

Key words: Cathedral; deformation; lead; roof; Washington Cathedral.

The Washington Cathedral, built in the English style, was given a lead roof. Under the hot Washington sun, it crept. This caused it to leak. E. W. Washburn, Chief Chemist of NBS, diagnosed the difficulty and suggested correction.

- 12679.** Shirk, J. S., Bass, A. M., **Absorption and laser-excited fluorescence of matrix-isolated CuO**, *J. Chem. Phys.* 52, No. 4, 1894-1901 (Feb. 15, 1970).

Key words: Absorption; laser-excited fluorescence; matrix isolation.

Absorption and laser-excited fluorescence spectra of CuO trapped in various matrices have been observed. The matrix data and previously observed gas-phase data are consistent with

	$\nu_{00}$ (matrix) ( $\text{cm}^{-1}$ )	$\nu_{00}$ (gas) <sup>5</sup> ( $\text{cm}^{-1}$ )	$\nu$ (matrix) ( $\text{cm}^{-1}$ )	( $\text{cm}^{-1}$ )
C		23 550		
$B^2\Sigma^?$	20 490	20 953	624	
$A(^2\Pi?)$	3 900	4 460	605	$(^2\Pi_{1/2}-^2\Pi_{3/2}=275)$
$X(^2\Pi)$	0	0	665	$(^2\Pi_{1/2}-^2\Pi_{3/2}\approx 200)$

for the lowest states of CuO. It is shown that the matrix-isolation technique can be used to "tune" an absorption into coincidence with a laser line in order to observe fluorescence. The vibrational relaxation of CuO in a solid matrix requires on the order of  $10^5$  vibrations.

- 12680.** Shirk, J. S., Bass, A. M., **Laser-excited fluorescence of matrix-isolated molecules**, *Anal. Chem.* 41, No. 11, 103A-107A (Sept. 1969).

Key words: Absorption; analytical methods; laser-excited fluorescence; matrix-isolation; molecular emission spectra; resonance fluorescence.

Matrix isolation and laser-excited fluorescence combined form highly specific, sensitive analytical techniques. The methods have great potential in solving analytical problems.

- 12681.** Swing, R. E., **Conditions for microdensitometer linearity**, *J. Opt. Soc. Amer.* 62, No. 2, 199-207 (Feb. 1972).

Key words: Coherence; microdensitometer.

A simple microdensitometer system is analyzed using the principles and analytical techniques of the theory of partial coherence. A specification of the physical conditions under which the instrument is linear is obtained, for incoherent illumination. The illuminating mutual intensity is then generalized, by the Van Cittert-Zernike theorem, and conditions on the partial coherence of the preslit illumination necessary for effective incoherence are determined. The new conditions determine a mode of linear operation for the microdensitometer for which an optical transfer function may be unambiguously defined.

- 12682.** Tauber, S. J., Rankin, K., **Valid structure diagrams and chemical gibberish**, *J. Chem. Doc.* 12, No. 1, 30-34 (1972).

Key words: Chemical structure diagrams; computer storage; display; geometric; grammar; input; labeled graph; overlap; topological; validation.

Chemical structure diagrams are considered as utterances in a written language. Two types of grammars are considered for this language: topological grammars which emphasize the connectivity of the diagrams and geometric grammars which emphasize the arrangement of the diagrams in a plane. The vocabulary associated with each grammar consists of entities like atomic symbols, numeric subscripts, and bond symbols. Examples are given of initialization, propagation, and terminalization rules from each type of grammar and of the application of such rules. The value of grammars for the validation of computer input and for generation of computer output are indicated. The hypothesis is presented that compact computer storage may become accessible via grammars.

**12683.** Tech, J. L., *Annual Reports of Observatories (National Bureau of Standards) 1970/71*, *Bull. Amer. Astron. Soc.* **4**, No. 1, 136-139 (1972).

Key words: Atomic spectra; cross section;  $f$ -values; molecular spectra; photoionization; rare-earths; review; spectroscopy; transition probabilities.

Research activities of astrophysical importance carried out by workers at the National Bureau of Standards during the past year are reviewed. A bibliography of publications is also presented.

**12684.** Tilford, S. G., Ginter, M. L., Bass, A. M., *Electronic spectra and structure of the hydrogen halides. The  $b\ ^3\Pi_i$  and  $C\ ^1\Pi$  states of HI and DI*, *J. Mol. Spectrosc.* **34**, No. 2, 327-340 (1970).

Key words: Absorption spectra; electronic spectra; high resolution; hydrogen halides; molecular constants.

The absorption spectra of HI and DI below 1900 Å have been photographed at high resolution. Analyses of the " $B$ "  $\leftarrow X$  and  $C \leftarrow X$  transitions show that the " $B$ " state is the  $^3\Pi_i$  component of a  $^3\Pi_i$  state (designated here as  $b$ ) and the  $C$  state is a  $^1\Pi$  state. Both  $b\ ^3\Pi_i$  and  $C\ ^1\Pi$  originate from the same  $\pi^3\sigma$  configuration, exhibit strong predissociations, and show some small Case  $c$  effects. The transition from approximately  $\Lambda$ ,  $S$  toward  $\Omega$ ,  $\omega$  coupling is discussed for the  $b$  and  $C$  states of hydrogen halides, HCl, DCl, HBr, DBr, HI, and DI. Effective molecular constants are presented for the  $b$  and  $C$  states of HI and DI.

**12685.** Vidal, C. R., Haller, F. B., *Heat pipe oven applications. I. Isothermal heater of well defined temperature. II. Production of metal vapor-gas mixtures*, *Rev. Sci. Instr.* **42**, No. 12, 1779-1784 (Dec. 1971).

Key words: Absorption and fluorescent cell; heat pipe oven; metal vapor-gas mixtures.

A concentric heat pipe oven is described, which serves as an oven with a highly homogeneous temperature distribution as required by such applications as crystal growing, thermal treatment of materials, and radiation standards. The design is simpler than conventional ovens with similar temperature stability and homogeneity. The temperature control is replaced by a pressure control. This device is used in a modification of the heat pipe oven that generates homogeneous mixtures of a vapor (such as a metal vapor) and an inert gas at well defined total pressure, partial pressure, temperature, and optical path length. All the features of the previously described heat pipe oven are maintained with the additional option that allows quantitative total and partial pressure measurements without relying on vapor pressure curves.

**12686.** Weise, W., Huber, M. G., Danos, M., *A microscopic description of the  $(\gamma, pn)$ -reaction*, *Z. Physik* **236**, 176-191 (1970).

Key words: Cluster expansion; high momentum com-

ponents; Jastrow wave function; photonuclear effect; quasideuteron effect; short range correlations.

The quasideuteron process has been investigated for photon energies  $40\text{ MeV} < E_\gamma < 160\text{ MeV}$  on the basis of a shell model picture modified by short range nucleon-nucleon correlations. It turns out that the cross section for the  $(\gamma, pn)$ -reaction depends sensitively on the details of the correlation function, i.e. on the exchange of high momenta between otherwise independently moving nucleons. The final state interaction has been consistently taken care of by using optical model wave functions for the outgoing nucleons. The results of the calculations for  $^{16}\text{O}$  indicate that precise measurements of the  $(\gamma, pn)$  cross section do contain information on the properties of the nuclear wave functions for small internucleonic distances.

**12687.** Weitzel, D. H., Cruz, J. E., Lowe, L. T., Richards, R. J., Mann, D. B., *Instrumentation for storage and transfer of hydrogen slush*, (Proc. 1970 Cryogenic Engineering Conf., June 17-19, 1970, Colorado Univ., Boulder, Colo.), Chapter in *Advances in Cryogenic Engineering*, K. D. Timmerhaus, ed., **16**, Paper No. F-1, 230-240 (Plenum Press, Inc., New York, N.Y., 1971).

Key words: Density; flow; hydrogen; instrumentation; slush hydrogen.

A program for development and testing of density and flow instrumentation for use in hydrogen liquid and liquid-solid mixtures (slush) is reviewed. Performance criteria are indicated along with experimental and analytical results which provide some basis for choices among the various candidate systems. The density work is nearing completion; the flow studies have not yet provided data beyond the demonstration of feasibility.

**12688.** Carpenter, B. S., *Quantitative applications of the nuclear track technique*, (Proc. Inter/Micro 71 Conf., London, England, Sept. 17-24, 1971), *Microscope* **20**, 175-182 (1972).

Key words: Boron; glasses; image analyzing system; liver; microscopy; neutron activation analysis; nitrogen; nuclear track technique; orchard leaves; steels; track etch method; uranium.

The nuclear track technique has been used since the early 1960's as a means of mapping the location of uranium and boron concentration in several matrices and in geochronology. This technique has now been applied to the quantitative determination of several elements that emit charged particles. The detector sample "sandwich" is exposed to the desired radiation source, fast or thermal neutrons, or high energy photons, and the charged particles emitted are registered in plastic detectors. The elements boron, lithium, nitrogen, thorium and uranium have been determined in various matrices; e.g. liver, orchard leaves, tomato leaves, blood, glass, soil, steel and minerals. The amount of material in these matrices is determined in three different ways, the absolute method, the method of standard additions and the comparative method. All three of these methods require that the plastic detectors be chemically etched and the resulting optically visible tracks are then counted with the aid of an image analyzing microscope.

**12689.** Carpenter, B. S., LaFleur, P. D., *Observing proton tracks in cellulose nitrate*, *Int. J. Appl. Radiat. Isotop.* **23**, 157-159 (1972).

Key words: Activation analysis; cellulose nitrate detectors; nitrogen; nuclear track technique; proton tracks.

Cellulose nitrate is used as a detector to observe monoenergetic proton tracks. These monoenergetic protons are produced from a  $^{14}\text{N}$  source placed in contact with the detector and ir-



radiated in a thermal-neutron flux. After irradiation the detectors are chemically etched to produce optically visible tracks.

- 12690.** Clough, R. B., **Mobile dislocation density and velocity in plastically deformed aluminum at room temperature**, *Scr. Met.* **6**, No. 4, 293-298 (1972).

**Key words:** Aluminum; dislocation velocity; mobile dislocation density.

Recently, Gillis and Hockett have calculated the Gilman drag stress in commercially-pure aluminum as a function of strain and temperature, basing their calculations on a model of yielding by Gillis and Gilman. The purpose of this note is to show that the Gillis-Gilman model used cannot properly be applied to yielding in aluminum at constant strain rate because it leads to an improbable dislocation velocity-stress relationship. Another more satisfactory model is proposed, and in addition it is pointed out that the entropy of plastic flow in aluminum is significant at 300 K.

- 12691.** Codling, K., Madden, R. P., **Resonances in the photoionization continuum of Kr and Xe**, *Phys. Rev. A* **4**, No. 6, 2261-2263 (Dec. 1971).

**Key words:** Autoionization; far ultraviolet; krypton; photoionization; resonances; xenon.

A total of 153 krypton resonances in the spectral region 500–337 Å, and 254 xenon resonances in the spectral region 600–375 Å are reported. The disposition of the detailed line lists are indicated. The analysis is very incomplete and will require detailed theoretical calculations to advance. In krypton, 45 resonances and in xenon, 56 resonances have been grouped into probable Rydberg series, for which classifications are suggested. In general, the resonances observed are due to the excitation of the inner subshell “s” electron ( $ns^2np^6 \rightarrow nsnp^6mp$ ) or to the excitation of two of the outer electrons simultaneously ( $ns^2np^6 \rightarrow ns^2np^4mll'$ ). These high-lying excited states autoionize, resulting in resonances with window-, asymmetric-, and absorption-type profiles. The detailed lists for the subshell “s” electron excitations are given.

- 12692.** Cooper, J. W., LaVilla, R. E., **“Semi-Auger” processes in  $L_{23}$  emission in Ar and KCl**, *Phys. Rev. Lett.* **25**, No. 26, 1745-1748 (Dec. 28, 1970).

**Key words:** Argon; configuration interaction; KCl; radiative process; two-electron processes; x-ray  $L_{23}$  emission.

X-ray emission studies in Ar and KCl due to formation of an  $L_{23}$  vacancy reveal a low-energy satellite below the main emission peak. Comparison with other data on related processes indicates that this satellite is due to two-electron effects (configuration interaction) in the final state of the emission process.

- 12693.** Coxon, B., **Application of internuclear, double-resonance techniques to carbohydrates. Detection of small coupling-constants**, *Carbohydrate Res.* **18**, No. 3, 427-442 (1971).

**Key words:** General Overhaus effect; internuclear double resonance; long-range coupling; magnetic equivalence factoring; spin-tickling; transient nutations; 6-deoxy- $\alpha$ -D-glucufuranose derivative.

6-Deoxy-1,2:3,5-di-O-isopropylidene- $\alpha$ -D-glucufuranose- $d_{12}$  (**1**- $d_{12}$ ) has been synthesized by an exchange reaction of its non-deuterated analog (**1**) with acetone- $d_6$ . The p.m.r. spectrum of **1**- $d_{12}$  at 90 MHz has been analyzed iteratively by means of a computer program for magnetic-equivalence factoring. Confirmation of the assignments of lines in the analysis has been investigated by proton-proton, internuclear, double-resonance (indor) techniques, which served also for the detection of a small long-range coupling-constant. Examples of indor spectra containing

general Overhauser effects, spin-tickling effects, or transient nutations are shown, and are discussed in relation to the experimental power-levels of the observing and double-resonance frequencies, and their sweep-rates. The mass spectra of **1** and **1**- $d_{12}$  are analyzed and compared.

- 12694.** Dodge, W. R., Murphy, J. J., **Ratio of the  $^4\text{He}(\gamma, p)$  and  $^4\text{He}(\gamma, n)$  cross sections**, *Phys. Rev. Lett.* **28**, No. 13, 839-843 (Mar. 27, 1972).

**Key words:** Differential cross section; electrodisintegration; isospin; light nuclei; photonuclear; ratio cross sections.

The  $^4\text{He}(\gamma, p)^3\text{H}$  and  $^4\text{He}(\gamma, n)^3\text{He}$  cross sections have been determined with a magnetic spectrometer in the energy interval of 30.0 to 51.8 MeV. We find that the average value of  $\sigma(\gamma, p)/\sigma(\gamma, n)$  is  $1.03 \pm 0.04$  in the above energy interval. The  $^4\text{He}(\gamma, p)$  cross section decreases from  $1.52 \pm 0.13$  mb at 31.7 MeV to  $0.36 \pm 0.03$  mb at 51.8 MeV.

- 12695.** Durst, R. A., Staples, B. R., Paabo, M., **Activity standards for ion-selective electrodes**, *Experientia Suppl.* **18**, 275-279 (1971).

**Key words:** Activity standards; clinical pH; electrodes; ion-selective electrodes; pH; potassium chloride; sodium chloride; standards.

Ion-selective electrodes, like the pH glass electrode, are finding growing use in various biomedical studies for monitoring the activities of ions such as  $\text{Ca}^{2+}$ ,  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Cl}^-$ ,  $\text{F}^-$ , etc. As in the case of the pH electrode, standards are also required for the reliable application of these sensors to complex biological fluids. Research is in progress to establish ionic activity scales and reference materials to permit the accurate use of ion-selective electrodes for biological and medical studies. At the present time, these investigations are concerned with aqueous standards and will progress to studies of these ions in mixed electrolyte systems and synthetic and real biologic fluids.

Studies are concurrently in progress to certify clinical pH standard buffers based on the tris/tris·HCl system [tris = tris(hydroxymethyl)aminomethane]. This buffer has been exhaustively studied to establish its behavior over wide temperature ranges and buffer ratios.

The standard reference materials resulting from these studies will serve the all-important purpose of calibrating ion-selective electrode analyzer systems for use in many areas of science and technology.

- 12696.** Eisen, H., Rosenstein, M., Silverman, J., **2.00-MeV electron depth-dose measurements in aluminum, copper and tin absorbers using a radiochromic dye film**, *Int. J. Appl. Radiat. Isotop.* **23**, 97-108 (Apr. 1972).

**Key words:** Absorbed energy; depth dose; electron energy deposition; radiation dosimetry.

The use of radiochromic dye films for electron dosimetry has been extended to absorbers with atomic numbers in the range 13–50. The depth-dose profiles in slab targets of aluminum, copper, and tin irradiated by a plane parallel 2.00-MeV electron beam are presented for incident beams at 0, 30, and 60 degrees with respect to the surface normal. Absolute energy deposition per unit fluence was determined by using calibrated films, a fluence measurement, and a stopping-power ratio correction. The results are compared to the ionization measurements of Nakai and to the theoretical calculations of Berger and Seltzer; all agree within 10 percent. The stopping-power ratio, necessary to convert dose in the dye film to absorber dose at that point, is determined three ways and the results compared. The three techniques range from a detailed computer transport calculation

yielding a variable stopping-power ratio with depth to the use of a constant stopping-power ratio obtained from tabulations. It is demonstrated that the use of the constant stopping-power ratio gives depth-dose distributions that differ by no more than 1-2 percent for aluminum, 3-5 percent for copper, and 4-8 percent for tin from the results obtained with the more rigorously evaluated stopping-power ratios.

**12697.** Fulmer, C. B., Toth, K. S., Williams, I. R., Handley, T. H., Dell, G. F., Callis, E. L., Jenkins, T. M., Wyckoff, J. M., **Photonuclear reactions in iron and aluminum bombarded with high-energy electrons**, *Phys. Rev. C* 2, No. 4, 1371-1378 (Oct. 1970).

Key words: Aluminum; GeV electrons; iron; photonuclear; production cross sections; radioactivity; spallation.

Previously reported evidence for photofission of iron is investigated by a more extensive study. Thin foils of iron were bombarded with beams of 1.5-, 3-, 5-, and 16-GeV electrons.  $\gamma$ -ray spectroscopy and radiochemical measurements were used to measure yields of radionuclides produced in the targets. The yields of 25 nuclides were measured for the bombarded iron foils; these include eight nuclides in the mass region  $22 \leq A \leq 35$ . A thin aluminum target was bombarded with 16-GeV electrons, and the yields of seven radionuclides were measured. The yield of  $^{24}\text{Na}$  in a thick iron target was measured as a function of target thickness and compared with that of radionuclides produced by cascade-evaporation reactions. The experimental evidence obtained in this series of experiments indicates that nuclides of mass  $< 35$  produced in the iron targets are the result of a fissionlike process. For cascade-evaporation reaction products, there is a decrease in the variation of yield with  $\Delta Z$  as the bremsstrahlung energy is increased.

**12698.** Gebbie, H. A., Bohlander, R. A., **Nonresonant cavity as a long path absorption cell**, *Appl. Opt.* 11, No. 4, 723-728 (Apr. 1972).

Key words: Absorption cell; far infrared; nonresonant cavity; spectroscopy.

We have constructed spherical specularly reflecting nonresonant cavities for use as absorption cells in far ir spectroscopy. A theory of their performance is developed and shown to be in agreement with experiment. An example is given of their use in a research program to ascertain the composition of water vapor. The essential advantage of these cells is that they give long pathlengths with high energy throughput.

**12699.** Geltman, S., **A high energy approximation: I. Proton-hydrogen charge transfer**, *J. Phys. B: At. Mol. Phys.* 4, No. 10, 1288-1298 (Oct. 1971).

Key words: Coulomb wave; Born approximation; electron; excitation; high energy; hydrogen; large angle; theoretical.

The proton-hydrogen ground state charge transfer process is studied in a first order approximation in which the proton-proton interaction is treated as belonging to the unperturbed part of the problem. This results in the appearance of a Coulomb wave rather than a plane wave in the final state of the  $T$  matrix. The result is a cross section which lies between the Brinkmann-Kramers and Jackson-Schiff results, with the high energy limit of  $0.810 \sigma_{BK}$ .

**12700.** Hayward, E., Gibson, B. F., O'Connell, J. S., **Consequences of isospin sum rules for photonuclear reactions**, *Phys. Rev. C* 5, No. 3, 846-852 (Mar. 1972).

Key words: Giant resonance; isoscalar; isospin; isosensor; isovector; photonuclear; sum rules.

Isospin sum rules for photonuclear reactions are derived; they relate the strengths of the two isospin components of the giant

resonance to the isoscalar, isovector, and isosensor radii of the nucleus. The connection between these radii and both the number and correlations of excess neutrons is discussed. A semiempirical formula for the fraction of the dipole strength in the  $T+1$  giant resonance is derived and various experimental data are discussed in the light of the results obtained using this equation.

**12701.** MacDonald, R. A., **Neutron scattering due to lattice distortion around point defects**, *J. Phys. F: Metal Phys.* 2, 209-218 (Mar. 1972).

Key words: Anisotropic elastic continuum; coherent scattering; differential scattering cross-section; elastic scattering; isotropic elastic continuum; lattice; local force model; long wavelength; neutron scattering; point defects; vacancy.

The distortions calculated from four different models of a vacancy, one discrete lattice model, two anisotropic continuum models and one isotropic continuum model are used to calculate the differential cross section for coherent elastic scattering of long wavelength neutrons by a single vacancy in copper. The results of the local force anisotropic continuum model and the isotropic continuum model are distinctly different from those of the discrete lattice and nonlocal force anisotropic continuum models. The effect of the distortion around the vacancy on the differential scattering cross section extends to at least 600 neighbouring atoms.

**12702.** Moore, G. A., **Recent progress in automatic image analysis**, *J. Microsc.* 95, Pt. 1, 105-118 (Feb. 1972).

Key words: Analysis of microstructures; automatic image analysis; Gestalt of a material; microarchitecture; patternness; scanning microscopes; television microscopes.

The utility of computing devices in stereology is evaluated with regard to three objectives. (1) Computer terminals permit easy and rapid prediction of 2-dimensional measurement distributions characteristic of any mathematically defined spatial structure. (2) The materials engineer can be satisfied by description of a Gestalt which characterizes the material as a whole and which can reasonably be presumed to control the behavior of the material in service. Six stereologically valid parameters are sufficient to define such a Gestalt. These are: volume fraction ( $V_V$ ), mean free path in the matrix ( $\bar{l}_a$ ), mean intercept width of particles ( $\bar{l}_p$ ), and measures of material variability, general anisotropy, and degree of patternness. Current scanner models are intrinsically suitable for these measurements but will benefit from standardized data outputs and improvements to increase measuring accuracy. (3) Microarchitectural observations such as counting and measuring, or identifying, individual object sections are inefficient in ordinary computers. Large program effort is required for limited machine intelligence and operating speeds are unsatisfactory. These machine operations are not yet competitive with human observers. New hardware systems appear to be necessary to economically simulate human processes of image recognition. Some proposed systems will be mentioned.

**12703.** Oneal, G., Jr., Harris, W. P., **Three-terminal cell for thin film dielectric measurements**, (Proc. Electrical Insulation and Dielectric Phenomena, Buck Hill Falls, Pa., Oct. 20-22, 1969), Chapter in *1969 Annual Report of the Conference Electrical Insulation and Dielectric Phenomena*, pp. 164-170 (National Research Council, National Academy of Sciences, Washington, D.C., 1970).

Key words: Dielectric constant; dissipation factor; electrical measurements; FEP fluorocarbon; polyethylene terephthalate; thin films; two fluid.

A new design of dielectric test cell for measuring the dielectric constant and dissipation factor of a thin film has been built. The



two fluid principle is used and agreement better than 1% in dielectric constant is obtained. Measurements on films as thin as 1.2  $\mu\text{m}$  (50 gage) and frequencies as high as 1 MHz are practicable. A byproduct of the calculation is the average thickness of the sample. Results of measurements on films such as "FEP" fluorocarbon and polyethylene terephthalate will be presented.

**12704.** Newman, M., **2-Generator groups and parabolic class numbers**, *Proc. Amer. Math. Soc.* **31**, No. 1, 51-53 (Jan. 1972).

**Key words:** Fuchsian groups; parabolic classes; 2-generator groups.

It is shown that if  $x, y$  are generators of the finite group  $G$  such that  $x^p = y^q = (xy)^n = 1$ , where  $p, q, n$  are integers  $> 1$ ,  $(p, q) = 1$ , and  $xy$  is of true order  $n$ , then the order  $\mu = nt$  of  $G$  satisfies  $n \leq pqt^p$ . This result is used to show that if  $F$  is a Fuchsian group of genus 0 generated by 2 elliptic elements of coprime order and with 1 parabolic class, then  $F$  possesses only finitely many normal subgroups having a given number of parabolic classes.

**12705.** Reichard, T. W., **Mechanical properties of insulating concretes**, Paper in *American Concrete Spec. Publ. SP 29, Lightweight Concrete*, pp. 253-316 (American Concrete Institute, Detroit, Michigan, 1971).

**Key words:** Cellular concrete; drying shrinkage; foam concrete; low density concrete; perlite concrete; thermal expansion; vermiculite concrete.

A description is given of a series of tests with insulating concretes of several types. The tests were designed to develop data for the purpose of determining: (1) Elastic properties and strength as a function of size and shape of specimen, curing method, density, and composition; (2) drying shrinkage; (3) thermally induced movements; and (4) the behavior of reinforced insulating concrete slabs under short-term and long-term loads.

Data are presented which show that although the relative strengths of various size specimens were affected by the curing method, the cubical specimen consistently showed a significantly higher strength than a cylindrical one with a height to diameter ratio of about two when their sizes are comparable.

There are significant differences in the drying shrinkages of 3 types of concretes and also in the shrinkages of the concretes made from the 3 brands of perlite.

**12706.** Reimann, C. W., **The single crystal spectra of dichlorotetrapyrazolenickel(II), dibromotetrapyrazolenickel(II), and hexapyrazolenickel(II) nitrate**, *J. Chem. Phys.* **74**, No. 3, 561-568 (Feb. 5, 1970).

**Key words:** Crystal spectra; pyrazole complexes; tetragonal molecular symmetry.

The single crystal spectra of hexapyrazolenickel(II) nitrate, dichlorotetrapyrazolenickel(II), and dibromotetrapyrazolenickel(II) from 6000 to 30,000  $\text{cm}^{-1}$  have been measured. The spectra of the halide complexes have been assigned on the basis of tetragonal molecular symmetry using the spectrum of hexapyrazolenickel(II) nitrate as a comparison. The tetragonal splittings in the first octahedral bands are considerably larger than observed in related complexes. These large splittings are related to low values of the effective  $Dq$  of the halide ions. Detailed crystallographic data are presented which show that the low effective field of the halide ions arises through an internal hydrogen bond interaction with the coordinated pyrazole molecules.

**12707.** Ritter, J. J., Coyle, T. D., Bellama, J. M., **Synthesis of ethynylboron halides**, *Chem. Commun.*, pp. 908-909 (1969).

**Key words:** Acetylenic boranes; ethynylchloroborane; ethynyldifluoroborane; organoboron halides.

The first examples of organoboron halides containing acetylenic groups have been prepared and characterized. Ethynylchloroborane,  $\text{HC}_2\text{BCl}_2$ , was obtained by irradiation of *cis*-bis(dichloroboryl)ethylene or *trans*-2-chlorovinyl-dichloroborane with a medium pressure mercury lamp (85% 2537 Å). The corresponding fluoride,  $\text{HC}_2\text{BF}_2$ , was prepared by the reaction of boron trifluoride with ethynyltrimethyltin. The compounds were characterized by infrared and mass spectroscopy and by cleavage of the ethynyl group with propionic acid to produce acetylene. In contrast to most known ethynylboranes, the new compounds are apparently stable as uncomplexed three-coordinate boron species.

**12708.** Roberts, J. R., Voigt, P. A., **The continuous emission from hydrogen at the bound-to-free transition regions**, *Proc. Xth Int. Conf. Phenomena in Ionized Gases, Oxford, England, Sept. 13-18, 1971*, p. 375 (1971).

**Key words:** Emission coefficient; hydrogen; hydrogen continuum; LTE; Stark broadening.

The continuous emission coefficient of a dense hydrogen plasma is appreciably modified by high density effects such as the lowering of the ionization potential and the merging of broadened higher lines to form a quasicontinuum. Close to a series limit, these effects become quite significant. A method for calculating the hydrogen emission coefficient near a series limit is proposed. The results of this method are in good agreement with the measured intensity distribution of a wall-stabilized hydrogen arc in the Balmer limit wavelength region of the spectrum.

**12709.** Rosenblatt, J. R., Filliben, J. J., **Randomization and the draft lottery**, *Science* **171**, 306-308 (Jan. 22, 1971).

**Key words:** Draft lottery; randomization; random numbers; random permutations.

Fifty "random permutations" were prepared for use by the Selective Service System as a basis for a two-stage randomization that preceded the lottery drawing on 1 July 1970. This report identifies the permutations used. It also gives the orders in which calendar dates and numbers were put into and drawn from two drums and the correlations between them.

**12710.** Rossmassler, S. A., **Federal information programs**, *Chem. Eng. Prog.* **67**, No. 11, 75-76 (Nov. 1971).

**Key words:** Chemical engineering information; data; information analysis centers; information systems; survey; technical information sources.

Many Federal Government programs can provide technical information and data useful to chemical engineers. Such material is available through government reports of completed work, professional journals, current project information systems, information analysis centers, specifications, the Patent Office, etc. Specialized information systems are evolving to make this information more accessible.

**12711.** Sengers, J. M. H. Levelt, Chen, W. T., **Vapor pressure, critical isochore, and some metastable states of  $\text{CO}_2$** , *J. Chem. Phys.* **56**, No. 1, 595-608 (Jan. 1, 1972).

**Key words:** Burnett method;  $\text{CO}_2$ ; coexistence curve; controlled clearance gage; critical exponent; critical isochore; critical region; metastable states pressure calibration; scaling law; vapor pressure.

An experimental method for obtaining precise *PVT* properties for gases in the critical region is described. Main features are

absence of noxious volumes, small height of sample volumes, precise temperature control, and high pressure sensitivity. Some results are presented for CO<sub>2</sub>. The 0 °C fixed point and the vapor-pressure curve have been measured and compared with literature values. Three liquid isochores including their metastable extensions into the two-phase region are also presented. The vapor-pressure data and pressures on the critical isochore above  $T_c$  are compared with the predictions of the thermodynamic scaling law and with those of a recently proposed extension of scaling. The equation of extended scaling fits the data between -2 and 46 °C with a standard deviation of  $1.5 \times 10^{-3}$  bar, for a "best" critical exponent  $\alpha = 0.09$ .

**12712.** Simmons, J. D., McDonald, J. K., *The emission spectrum of AlN*, *J. Mol. Spectrosc.* **41**, 584-594 (1972).

Key words: AlN; electronic spectrum; emission spectrum; high resolution; hyperfine broadening.

A new system of emission bands has been observed in the visible region of the spectrum. The bands exhibit the characteristic rotational structure of a  $^3\Pi_i - ^3\Pi_i$  electronic transition. Rotational analysis and isotopic studies of these bands indicate that the carrier of the spectrum is the species AlN. The rotational analyses of the (0 - 0) and (0 - 1) Al<sup>14</sup>N bands yield the following rotational constants, band origins, and lower state vibrational frequency  $\Delta G''_{1/2}$

$$\nu_0(0 - 0) = 19727.37 \text{ cm}^{-1}; \nu_0(0 - 1) = 18980.44 \text{ cm}^{-1};$$

$$B_0' = 0.5811 \text{ cm}^{-1}; B_0'' = 0.5702 \text{ cm}^{-1}; B_1' = 0.5646 \text{ cm}^{-1};$$

$$A_0' \cong -23 \text{ cm}^{-1}; A_0'' \cong -33 \text{ cm}^{-1}; A_1'' \cong -34 \text{ cm}^{-1};$$

$$\Delta G''_{1/2} = 746.8 \text{ cm}^{-1}.$$

The rotational analysis of the (0 - 0) Al<sup>15</sup>N band yields:

$$\nu_0(0 - 0) = 19727.13 \text{ cm}^{-1};$$

$$B_0' = 0.5559 \text{ cm}^{-1}; B_0'' = 0.5454 \text{ cm}^{-1};$$

$$A_0' \cong -21 \text{ cm}^{-1}; A_0'' \cong -31 \text{ cm}^{-1}.$$

An interesting pattern of sharp and broadened lines observed throughout the bands will be discussed in terms of unresolved nuclear hyperfine splittings.

**12713.** Taylor, J. K., Ed., Alvarez, R. A., Paulson, R., Rains, T. C., Rook, H. L., *Interaction of nitrilotriacetic acid with suspended and bottom material*, *Water Pollution Control Research Series 16020 GFR 07-71—Environmental Protection Agency (Progress Report)*, pp. 1-31 (July 1971).

Key words: Detergent; nitrilotriacetic acid; water pollution.

An experimental investigation was made of the possible interaction of residual concentrations of nitrilotriacetic acid in surface waters with metallic elements contained in sediments and bottom materials. Samples of bottom materials from typical bodies of surface waters were analyzed for their major, minor, and trace constituents. Eight representative samples of these were equilibrated with distilled water and with water containing 20 ppm of NTA and the resulting solutions were analyzed by three analytical techniques. Elements showing essentially no increased solubility in the presence of NTA were: barium, antimony, molybdenum, strontium, chromium, silver, tin, iron, lead, cadmium, copper, and mercury. Elements showing small increases in solubility were: nickel, zinc, manganese, and cobalt. Calcium and magnesium concentrations were increased somewhat above their normal relatively high concentrations.

This report was submitted in fulfillment of Project No. 16020 GFR under sponsorship of the Water Quality Office, Environmental Protection Agency.

**12714.** Thom, H. C. S., Marshall, R. D., *Wind and surge damage due to hurricane Camille*, *J. Waterways, Harbors, Coastal Eng. Div. Proc. Amer. Soc. Civil Eng.* **WW2**, No. 8144, 355-363 (May 1971).

Key words: Coastal engineering; damage; hurricanes; ocean waves; probability theory; storms; storm surges; wind.

The wind speeds in hurricane Camille are evaluated to provide a structural engineering interpretation. These are compared to published design winds for the area. Similar evaluation is made of the storm surge heights. A new method of probability analysis is applied to the historical surge data for Biloxi. Surveys of the storm and surge damage are considered with reference to actual wind speeds and design values in various parts of the storm area.

**12715.** von Busch, F., Dunn, G. H., *Photodissociation of H<sub>2</sub><sup>+</sup> and D<sub>2</sub><sup>+</sup>: Experiment*, *Phys. Rev. A* **5**, No. 4, 1726-1743 (Apr. 1972).

Key words: D<sub>2</sub><sup>+</sup>; experiment; H<sub>2</sub><sup>+</sup>; ionization; photodissociation; vibrational state populations.

Measurements are reported of the cross sections for photodissociation of H<sub>2</sub><sup>+</sup> and D<sub>2</sub><sup>+</sup> at 21 wavelengths ranging from 2472 to 13,613 Å. The measurements are compared with theory using normalized Franck-Condon factors for the vibrational populations of the ions. Deviations are found, which are interpreted as a failure of this latter approximation. A least-squares analysis of the data yields vibrational-state populations different from simple Franck-Condon factors and alleged to be those characteristic high-energy electron-impact ionization of H<sub>2</sub> and D<sub>2</sub>. Interpretation of the data using a mechanism requiring that a fraction of the ions formed by electron impact be generated via the autoionization channel can qualitatively lead to the observations of this experiment. However, such an explanation would require about 2/3 of all H<sub>2</sub><sup>+</sup> and D<sub>2</sub><sup>+</sup> to be formed via autoionization—a seemingly unrealistic requirement. Interpretation of the data in terms of a variation with internuclear separation of the electronic matrix element involved in the electron-impact ionization process shows that a matrix element varying as  $Q_e(r) = 1 + 0.56(r_{a.u.} - 0.99)^2$  can lead to the experimentally deduced populations of both H<sub>2</sub><sup>+</sup> and D<sub>2</sub><sup>+</sup>. This latter interpretation is favored, though one cannot rule out the former or some combination of the two. The data and interpretation are consistent with other related experiments.

**12716.** Scheer, M. D., Klein, R., *The addition of O(<sup>3</sup>P) to olefins. The nature of the intermediate*, *J. Phys. Chem.* **74**, 2732-2733 (1970).

Key words: Intermediate; olefins; oxygen atoms.

The currently available evidence, particularly that obtained at low temperatures, tends to support the Klein-Scheer planar intermediate for the reaction of ground state O atoms with olefins. This structure subsequently undergoes a set of concerted rearrangements in which a given group migration and oxygen atom localization occurs simultaneously to produce the final reaction products. Since electron spin is *not* conserved in the total reaction, the argument that a "triplet biradical" must first be formed before rearranging to singlet products is not compelling. The path by which the intermediate for this process rearranges to form the final products probably involves both energy and steric effects whose details have yet to be entirely elucidated. The spin relaxation process may ultimately prove to be only a minor barrier to the successful completion of these complex intramolecular rearrangements.

**12717.** Yakowitz, H., Ballantyne, J. P., Munro, E., Nixon, W. C., *The cylindrical secondary electron detector as a voltage measuring device in the scanning electron microscope*, *Proc. 5th An-*



**Key words:** Computer aided design; contamination resters; electron trajectories; scanning electron microscopy; secondary electron detection; voltage contrast.

Voltage effects at a specimen surface have been investigated using secondary electron detectors in which several electrodes can be independently biased with respect to the specimen. Different electrode arrangements and bias conditions were tested. Electron trajectories and equipotentials within the cylindrical region were computed for various arrangements of electrodes and electrode bias values. Using these calculations, a detector of equal radius and height, 23mm, was built. With this detector conditions were found where the collected secondary electron current varied by over 30% per volt in the range - 5 volts to + 8 volts of specimen bias. Results for various conditions of electrode bias are given. The observed voltage response arises primarily from the spread of the electron trajectories as a function of secondary electron energy.

**12718.** Ballard, D. B., **Comparison and evaluation of specimens for resolution standard**, *Proc. 5th Annual Scanning Electron Microscope Symp., ITT Research Institute, Chicago, Ill., Apr. 1972, Part 1, pp. 121-128 (1972).*

**Key words:** Resolution; resolution specimens; secondary emission; SEM; specimen criteria.

A need exists for resolution test specimens for the SEM. The criteria for such specimens are restrictive and depend on various electron beam-specimen interactions. These criteria include, secondary emission, contrast, low contamination, beam and vacuum resistance, variable spacing, tapered edges, coating, rigid structure, beam deflection, vacuum cleanliness, known surface topography, use and storage, cost and availability, and stigmator adjustment.

Some of the commonly used specimens to demonstrate resolution are silver, iron oxide, gold deposit, aluminum-tungsten alloy, pearlite, gallium arsenide-gallium arsenide phosphide, thorium dioxide tetraoxide crystals, graphite, magnetic recording tape, zinc oxide, opal, latex spheres and marine micro-fossils. No single sample meets all the criteria though the finely spaced dendritic structure of the metallic Al-W sample satisfies most specimen requirements except for independent magnification calibration. An accurate magnification standard is now required so that resolution of a particular SEM can be determined accurately.

**12719.** Rosenstein, M., McLaughlin, W. L., Silverman, J., **Energy deposition of electron beams in insulating materials**, (Proc. 4th Int. Conf. on Electron and Ion Beam Science and Technology, Los Angeles, Calif., May 1970), Chapter in *Electron and Ion Beam Science and Technology, 4th International Conference*, R. Bakish, ed., pp. 591-604 (The Electrochemical Society, New York, N.Y., 1970).

**Key words:** Charge deposition; depth dose; dielectrics; dose distribution; dosimetry; dye film dosimeter; electron beams; polystyrene; radiochromic dye.

Experimental depth-dose curves were obtained for semi-infinite thicknesses of ordinary and conducting polystyrene, irradiated in air by a 1.5-MeV electron beam in the dose range 5 to 20 Mrad. Radiochromic dye films were used as spatial dosimeters. By using a calibration of optical density versus dose, a microdensitometric reading of the irradiated dye films gave continuous depth-dose curves. No difference was observed between the depth-dose curves for the ordinary polystyrene and conducting polystyrene at absorbed dose rates between 2.5 and 10

Mrad/min. Within the limits of uncertainty for the present experiment, the results are in agreement with theoretical and experimental depth-dose data for 1.5-MeV electrons in polystyrene. Under the conditions studied, trapped charge does not measurably perturb the energy deposition of electrons in polystyrene.

**12720.** Powell, C. J., **Structure on the high-energy side of the  $KL_{23}M$  Auger peak from solid aluminum: Internal photoemission**, *Appl. Phys. Lett.* 20, No. 9, 335-337 (May 1, 1972).

**Key words:** Aluminum; Auger-peak; secondary-electron energy distribution; x-ray photoemission.

Some weak structure on the high-energy side of the  $L_{23}MM$  Auger peaks for Al and Si has been recently interpreted as being possibly due to the simultaneous decay of an inner-shell vacancy and a volume plasmon. It is shown here that similar structure due to multiple ionization is to be expected and that photoemission caused by internally generated x rays can be observed if the fluorescent yield is not too small. Relatively strong structure of the latter type has been observed in the secondary-electron energy distribution of evaporated Al on the high-energy side of the  $KL_{23}M$  Auger peak.

**12721.** Carter, G. C., Weisman, I. D., Bennett, L. H., Watson, R. E., **The  $AuAl_2$ - $AuGa_2$ - $AuIn_2$  problem: Knight shifts and relaxation times in their pseudobinary alloys**, *Phys. Rev. B* 5, No. 9, 3621-3638 (May 1, 1972).

**Key words:** Alloys; aluminum; gallium; gold; indium; intermetallic compound; Knight shift; relaxation time; soft x-ray spectroscopy; x-ray photoemission spectroscopy.

The nuclear-magnetic-resonance (NMR) and susceptibility behavior of the intermetallic compound  $AuGa_2$  differs anomalously from the isolectric and isostructural compounds  $AuIn_2$  and  $AuAl_2$ . In an effort to test and extend the explanation offered by Jaccarino et al. and by Switendick and Narath, spin-lattice relaxation times and Knight shifts have been measured as a function of temperature and composition for the  $AuAl_2$ - $AuGa_2$ ,  $AuAl_2$ - $AuIn_2$ , and  $AuGa_2$ - $AuIn_2$  pseudobinary alloy systems. At high temperature, the solute X (Al, In, Ga) resonance properties are dominated by the host. Satellite resonances are observed with temperature dependences differing from the main resonance. The results are partially explainable on the basis of an average-band model and partially on a local atom model. The role of the Au d bands is discussed. Metallurgical results on alloying are obtained using the NMR data.

**12722.** Shapiro, H. M., Bryan, S. D., Lipkin, L. E., Stein, P. G., Lemkin, P. F., **Computer-aided microspectrophotometry of biological specimens**, *Exp. Cell Res.* 67, No. 1, 81-89 (July 1971).

**Key words:** Cytochemistry; histochemistry; image processing; laboratory automation; microscopy; spectrophotometry.

A scanning microspectrophotometer controlled by a small digital computer is used to produce data which is analysed using a larger, remote digital computer. Programs have been written for the smaller machine to permit automatic scanning of a large number of preselected fields. Other programs, written for the larger machine, enable the experimenter to pick out cells in a scan field and measure their size and optical density, or automatically locate and measure cells within a scan field, and generate statistical analyses of size and optical density measures for a number of cells. The further implications of this work for cytochemistry are discussed.

12723. Semmelroth, C. C., **Adjustment of the Munsell-value and  $W^*$ -scales to uniform lightness steps for various background reflectances**, *Appl. Opt.* 10, No. 1, 14-18 (Jan. 1971).

Key words: Background effect; Munsell-value; reflectance.

For background reflectances taken equal to, or slightly lower than, the specimen reflectances, the Munsell-value,  $V$ , and the CIE 1964,  $W^*$ , scales are found to be essentially linear with a power formulation for lightness previously shown to accord with lightness-spacing data for a wide variety of specimen and background reflectances. Adjustments required to make the Munsell-value function accord precisely with the power formulation for this background condition are all less than 0.2 of a Munsell-value step between 1/ and 9/. The power formulation is used to construct a table to show in Munsell terms the influence of background reflectance on perceived lightness for all combinations of specimen and background reflectance including Takasaki crispening for specimen reflectance approaching that of the background.

12724. Bender, P. L., Dicke, R. H., Wilkinson, D. T., Alley, C. O., Currie, D. G., Faller, J. E., Mulholland, J. D., Silverberg, E. C., Plotkin, H. H., Kaula, W. M., MacDonald, G. J. F., **The lunar laser ranging experiment**, (Proc. Conf. on Experimental Tests of Gravitational Theories, Pasadena, Calif., Nov. 1970), *JPL Technical Memo 33-499*, pp. 178-181 (Jet Propulsion Laboratories, Pasadena, Calif., Nov. 1971).

Key words: Gravity; laser; lunar motion; moon; relativity.

The emplacement of the Apollo II retro-reflector package on the lunar surface has made possible very accurate measurements of the lunar distance. A continuing program of range measurements to the package at nearly all phases of the moon is being carried out by the McDonald Observatory under NASA support. Returned signals have also been obtained by the Pic du Midi Observatory in France and by the AFCRL Lunar Laser Observatory near Tucson, Arizona. It is hoped that several other lunar ranging stations will be in operation within the next year or two, including ones in Japan, Hawaii, Russia, and the southern hemisphere.

12725. Semmelroth, C. C., **Prediction of lightness and brightness on different backgrounds**, *J. Opt. Soc. Amer.* 60, No. 12, 1685-1689 (Dec. 1970).

Key words: Color; vision.

Two psychophysical responses to surface or self-luminous stimuli are hypothesized. A response to the luminance of the stimulus ( $\alpha$ ) and a response to the luminance difference between the stimulus and its surround ( $\beta$ ) are both considered to be power functions. Lightness or brightness is taken to be an additive or subtractive combination of these two responses ( $\alpha \pm K\beta$ ) depending on whether the surround is darker or brighter than the stimulus, respectively. This model is shown to produce a quantitatively adequate explanation of Takasaki's data on crispening. An attempt is made to use this formulation to fit scaling data from previous magnitude-estimation and partitioning studies of lightness and brightness in which different results have been obtained from different backgrounds. Data from matching experiments that involve different backgrounds for the comparison and standard stimuli are also analyzed by means of the same formulation. The model is compared with the Adams-Cobb-Judd formulation of background effect on lightness, the Takasaki empirical formula for crispening, and Stevens's power-law formulation for brightness and lightness.

12726. Mahler, R. J., Phelan, R. J., Jr., Cook, A. R., **High  $D^*$ , fast, lead zirconate titanate pyroelectric detectors**, *Infrared Phys.* 12, 57-59 (1972).

Key words: Infrared; pyroelectric; room temperature detector.

Large area PZT detectors with  $D^*$  (500 K, 1, 1.) =  $7 \times 10^8$  cm  $\text{Hz}^{1/2}/\text{W}$  and fast detectors with a response time of at least 5 nsec have been fabricated. The pyroelectric coefficient of  $27 \text{ nC/cm}^2$  K and a materials figure of merit of  $2.8 \times 10^{-9} \text{ C cm/J}$  have been measured for these devices.

12727. Mulholland, J. D., Alley, C. O., Bender, P. L., Currie, D. G., Dicke, R. H., Faller, J. E., Kaula, W. M., MacDonald, G. J. F., Plotkin, H. H., Wilkinson, D. T., **Preliminary results of laser ranging to a reflector on the lunar surface**, (Proc. 13th Plenary Meeting of COSPAR, Leningrad, May 1970), *Space Research XI*, 97-104 (Academie-Verlag, Berlin, 1971).

Key words: Celestial mechanics; geophysics; laser; lunar ephemeris; selenology.

The first Lunar Ranging Experiment (LURE) retroreflector array was placed on the lunar surface during the Apollo 11 mission. Prior to this event, a special high-precision lunar ephemeris (designated LE 16) was developed by means of a composite numeric/analytic process, so as to provide more accurate predictions for use at the telescope. First returns were observed at the Lick Observatory on 1 August 1969 and at the McDonald Observatory shortly thereafter. The observing program is to continue for several years. Preliminary use of these data consists of their comparison with the LE 16 ephemeris, preparatory to a differential correction of the lunar elements. Present indications are that the ephemeris must undergo order-of-magnitude improvements before the full power of the laser data can be utilized. Other parameters in the predictive process are also capable of being corrected; an improvement in the coordinates of the Lick Observatory 120-inch telescope is already indicated.

12728. Sengers, J. V., **Triple collision effects in the transport properties for a gas of hard spheres**, (Proc. Symp. on Kinetic Equations, Cornell University, Ithaca, N.Y., 1969), Paper C-1 in *Kinetic Equations*, R. L. Kiboff and N. Rostoker, eds., pp. 137-193 (Gordon and Breach, New York, N.Y., 1971).

Key words: Collision integrals; hard spheres; thermodynamic conductivity transport properties; triple collisions; viscosity.

A study is made of the effect of successive correlated binary collisions on the transport properties of gases. In particular, triple collision transport integrals are derived for the thermal conductivity and viscosity of a gas of hard spheres. Preliminary numerical estimates for these collision integrals allow us to make an assessment of the contributions from the various triple collision events.

12729. Danos, M., **Baryon resonances in the nuclear ground state: How about double counting?**, (Proc. 3d Int. Conf. High-Energy Physics and Nuclear Structure, Columbia University, New York, N.Y., Sept. 7-12, 1969), Chapter in *High-Energy Physics and Nuclear Structure*, pp. 811-815 (Plenum Press, New York, N.Y., 1970).

Key words: Baryon resonances; exchange currents; nuclear magnetic moments; nucleons;  $\pi$ -mesons; relativistic nuclear physics.

In a relativistic treatment of nuclei one encounters serious problems of double or multiple counting. They are associated with the existence of baryon and meson resonances. A procedure is described for overcoming these difficulties.

12730. Flynn, D. R., **Considerations in launching effective noise control programs**, (Proc. EASCON 1971 Conf., Oct. 6-8,



1971, Washington, D.C.), *IEEE Trans. Aerosp. Electron. Syst.*, pp. 53-59 (Nov. 1971).

**Key words:** Acoustics; environmental control; measurement; noise; pollution; sound.

Measurement plays a pervasive role in assessing the consequences of noise, its effects and control. Both the assessment of noise problems and the assessment of alternative strategies for noise abatement and control ultimately rest on accurate, reliable, and relevant measurement capability. Accurate measurement is required in order to ascertain the effects of a given noise exposure, to establish trends in noise exposure, to permit selection of cost-effective solutions, to monitor the effectiveness of control programs, and to provide the factual (measurement) basis for legal regulation. While considerable information is presently available regarding measurement and monitoring of noise, further work which will lead to more accurate or less expensive measurement methods is clearly needed. This paper will include a brief discussion of the research needs in assessment of the effects of noise on people, in characterization of the noise generation or transmission characteristics of various products or systems, and in development of meaningful correlations between noise exposure and the related human responses.

**12731.** Nimeroff, I., **The psychology of color**, *Amer. Paint J.*, pp. 65-70 (Jan. 11, 1971).

**Key words:** Color aesthetics; color vision; psychology of color.

In recent years there has been an increase in the attention that is being given by scientists, particularly psychologists, to a field of study called "the psychology of color." Selected language that associates color with emotions, with neuroses and psychoses, with health and illness, with human endeavors, with aesthetics, and the like, are some of the topics that have been and are being studied. Some of these studies are reported here. The mental associations with color present a practical difficulty in that there is such great disparity in language usage and association among individuals and among groups of people. Other topics, more subject to conventional quantitative study, are also related to psychological effects of color. These include: uniform color spacing, color harmony, color naming or ordering, and color metamerism. If we can gather sufficient information about the psychology of color and the color of man's environments, we may look forward to a time when we can devise ideal decor for living and working quarters.

**12732.** Yule, H. P., **Study of gamma-ray spectrum distortion by mathematical smoothing**, *Anal. Chem.* **44**, No. 7, 1245-1249 (June 1972).

**Key words:** Digital data smoothing; digital filtering; distortion; gamma-ray spectra; mathematical smoothing.

Removal of statistical scatter from gamma-ray spectra is a considerable aid in the computerized reduction of spectral data. Application of mathematical filters to the data may result in erroneous results due to distortion introduced by the filter. Such distortion is often difficult to detect and even more difficult to measure. In the present paper, repeated filtering, or smoothing, is applied to different spectral situations to obtain indications of the amount of distortions introduced by smoothing. It is concluded that filtering one time, the usual number of smoothing, introduces little distortion in most cases, although overlapping peaks may suffer some distortion.

**12733.** Rook, H. L., Gills, T. E., LaFleur, P. D., **Method for the determination of mercury in biological materials by neutron activation analysis**, *Anal. Chem.* **44**, No. 7, 1114-1117 (June 1972).

**Key words:** Activation analysis; biological; environment; mercury; Standard Reference Material.

A method is described for the determination of mercury in a variety of matrices. Three significant improvements over currently used procedures have been achieved: The procedure has a minimum of chemical manipulations, thereby minimizing technique related errors; the radiomercury separation is quantitative, thus eliminating unnecessary errors involved in the determination of chemical yields; the procedure is based on a simple combustion separation of radiomercury allowing the same technique to be used on a wide variety of matrices. The method was tested using radiotracer experiments and by analyzing samples of flour and coal which had been independently analyzed. The procedure has been subsequently used to determine the mercury concentration of two new Standard Reference Materials being offered by the National Bureau of Standards.

**12734.** Rook, H. L., **Rapid, quantitative separation for the determination of selenium using neutron activation analysis**, *Anal. Chem.* **44**, No. 7, 1276-1278 (June 1972).

**Key words:** Biological; neutron activation analysis; selenium; standard.

The role selenium plays in the biochemistry of higher animals is complex and as yet, ill defined. A prerequisite for definitive studies is a sensitive, accurate analytical procedure for selenium. Relatively few analytical techniques fulfill both criteria of sensitivity and accuracy in biological and environmental matrices. This work describes a simple, effective method for the determination of selenium by neutron activation analysis using a combustion separation of volatile elements followed by liquid nitrogen freezing.

**12735.** Yates, J. T., Jr., Madey, T. E., **The adsorption of methane by tungsten (100)**, *Surface Sci.* **28**, 437-459 (1971).

**Key words:** Adsorption; field emission; methane; physical adsorption; single crystal; tungsten; work function.

The adsorption of methane by the (100) plane of tungsten has been studied using flash desorption and work function methods. It has been found that CH<sub>4</sub> adsorbs to appreciable coverage as an undissociated molecular species at ~ 100 K. The activation energy for first order desorption from this state is 6.9 kcal/mole (0.30 eV/molecule). This observed binding energy is greater than expected for dispersion forces alone, and added contributions to the binding energy are discussed. An observed work function of - 0.34 eV on adsorption of CH<sub>4</sub> is consistent with the presence of a physically adsorbed CH<sub>4</sub> layer.

Related studies of CH<sub>4</sub> adsorbed on a tungsten field emission tip demonstrate that adsorption of CH<sub>4</sub> proceeds rapidly at 77 K, but is negligible at 300 K. At tungsten temperatures above 1200 K in 10<sup>-5</sup> torr of CH<sub>4</sub>, decomposition of the CH<sub>4</sub> to form a carbon layer occurs.

It is postulated that at elevated temperatures and at high CH<sub>4</sub> pressures the physically adsorbed state may be sufficiently populated to serve as a source of adsorbed CH<sub>4</sub> species which undergo activated surface decomposition, leading eventually to surface carbides.

**12736.** Madey, T. E., **Adsorption and displacement processes on W(111) involving CH<sub>4</sub>, H<sub>2</sub>, and O<sub>2</sub>**, *Surface Sci.* **29**, 571-589 (1972).

**Key words:** Binding energy; chemisorption; displacement; hydrogen; methane; oxygen; tungsten; work function.

Adsorption and displacement processes involving CH<sub>4</sub>, H<sub>2</sub>, and O<sub>2</sub> on the (111) surface of tungsten have been examined using the thermal desorption method in conjunction with mass

spectrometry and work function changes. Methane is physically adsorbed on W(111) at  $T \sim 125$  K and desorbs with a binding energy of 8.0 kcal/mole. Neither adsorption nor decomposition of  $\text{CH}_4$  is observed at 300 K on W(111). Hydrogen is chemisorbed on W(111); 4 atomic binding states having desorption energies from 12 kcal/mole to 31 kcal/mole are observed. The influence of oxygen on the binding of both  $\text{H}_2$  and  $\text{CH}_4$  has been examined. Oxygen specifically blocks the adsorption of certain hydrogen binding states; oxygen causes an increase in the  $\text{CH}_4$  binding energy to  $\sim 10$  kcal/mole. Coadsorption of hydrogen and  $\text{CH}_4$  also exhibits site specificity.

- 12737.** Comeford, J. J., **The spectral distribution of radiant energy of a gas-fired radiant panel and some diffusion flames**, *Combust. Flame* **18**, 125-132 (1972).

Key words: Diffusion flames; emission spectra; flame spectra; infrared spectra; radiant test panel; radiant test sources.

Measurements were made of the spectral distribution of energy from radiant sources employed in standard test methods of flammability. Radiant sources examined were a gas-fired radiant panel employed in ASTM Test E-162 and the electric heater employed in the Smoke Chamber Test. To afford a basis for comparison, the emission spectra of several diffusion flames in air were measured. The energy distribution of the flames occurred essentially in two narrow wavelength intervals corresponding to emission of carbon dioxide at  $4.4 \mu\text{m}$  and water at  $2.7 \mu\text{m}$ . Luminous diffusion flames containing large amounts of incandescent carbon, such as occur from the combustion of acetylene-in-air, show a blackbody background continuum with  $\text{CO}_2$  and  $\text{H}_2\text{O}$  emission peaks superimposed on the continuum. The radiant test sources exhibited an energy distribution approximating that of a blackbody with atmospheric  $\text{CO}_2$  and  $\text{H}_2\text{O}$  absorptions superimposed. The gas-fired radiant panel in addition showed a significant emission peak at  $4.4 \mu\text{m}$  due to excited  $\text{CO}_2$ .

- 12738.** LaVilla, R. E.,  **$K\alpha$  emission spectrum of gaseous  $\text{N}_2$** , *J. Chem. Phys.* **56**, No. 5, 2345-2349 (Mar. 1, 1972).

Key words: Electron bombardment; lead myristate analyzing crystal; M. O. correlation; nitrogen  $K$  emission spectrum; resonance radiation; x-ray emission.

The nitrogen  $K\alpha$  emission spectrum excited by electron bombardment of nitrogen gas was obtained on a single planar crystal spectrometer with photon counting. The experimental profile is in fair agreement with a calculated profile based on molecular orbital theory and the single vacancy states measured by x-ray photoelectron spectroscopy. Evidence is presented to suggest that some of the emission intensity on the high-energy side of the main peak is due to "resonance radiation." To fix the energy scale of the spectrum, the effective  $2d$  spacing of the analyzing lead myristate crystal was experimentally determined.

- 12739.** Okabe, H., **Photodissociation of  $\text{OSCl}_2$  in the vacuum ultraviolet; the heat of formation of  $\text{SO}$** , *J. Chem. Phys.* **56**, No. 7, 3378-3381 (Apr. 1, 1972).

Key words: Heat of formation;  $\text{OSCl}_2$ ; photodissociation;  $\text{SO}$ ; vacuum ultraviolet.

The photodissociation of  $\text{OSCl}_2$  at the Kr (1165-, 1236-Å) lines has resulted in the production of  $\text{SO } A^3\Pi$ ,  $B^3\Sigma$ . The threshold energy of incident photons to produce the reaction,



was  $9.41 \pm 0.03$  eV from which  $\Delta H_f^\circ(\text{SO}) = 1.3 \pm 0.7$  kcal/mole is derived. The  $I_f/I_0$ -vs-incident wavelength curve shows many diffuse bands found in the absorption spectrum of  $\text{OSCl}_2$  indicating that the process is predissociative. Various other

methods to obtain  $\Delta H_f^\circ(\text{SO})$  are compared. It is concluded that the best value is  $1.3 > \Delta H_f^\circ(\text{SO}) > 0.8$  kcal/mole.

- 12740.** Stephenson, N. C., Roth, R. S., **The crystal structure of the high temperature form of  $\text{Ta}_2\text{O}_5$** , *J. Solid State Chem.* **3**, 145-153 (1971).

Key words: Crystallographic shear; crystal structure; high temperature  $\text{Ta}_2\text{O}_5$ ; nonstoichiometric.

The structure of the high temperature form of  $\text{Ta}_2\text{O}_5$  can be stabilized by doping with 2 mole%  $\text{Sc}_2\text{O}_3$  and single crystals have been prepared from a  $\text{Ta}_2\text{O}_5$ - $\text{Sc}_2\text{O}_3$  (98:2) composition by the Czochralski technique. The crystal system which at first appeared to be body-centered tetragonal has been determined to be face-centered monoclinic, space group  $C2$  with  $a = 35.966$  Å,  $b = 3.810$  Å,  $c = 3.810$  Å,  $\beta = 96^\circ 7'$ . Least-squares refinement cycles reduced the reliability index  $R$  to 0.089.

The structure consists of  $\alpha\text{UO}_3$ -type blocks in which each tantalum atom is surrounded by a pentagonal bipyramid of oxygen atoms. These blocks are infinite in two directions and are separated from similar blocks along a third direction by shear planes. In the vicinity of these shear planes the tantalum atoms are surrounded by distorted octahedral coordination polyhedra.

It is believed that the stabilizing effect of the  $\text{Sc}_2\text{O}_3$  impurity is due to an increase in the concentration of shear planes. Random shear planes (Wadsley defects) are introduced at approximately  $300$  Å intervals along the large axis by doping with a substance ( $\text{Sc}_2\text{O}_3$ ) which has cations (Sc) large enough to substitute for the host (Ta) but a lower oxygen:metal ratio than the host compound ( $\text{Ta}_2\text{O}_5$ ).

- 12741.** Schrack, R. A., Heaton, H. T., II, Schwartz, R. B., **Suppression of after-pulsing in the type 58AVP photomultiplier**, *Nucl. Instr. Methods* **77**, 175-176 (1970).

Key words: After-pulse; gamma flash; neutron; photomultiplier; pulse; time-of-flight.

A technique for eliminating the after-pulse observed in photomultipliers after intense light pulses is described.

- 12742.** Thompson, B. A., Lutz, G. J., **Characterization of ancient bronze artifacts by neutron and photon activation analysis**, *Radiochem. Radioanal. Lett.* **9**, No. 5-6, 343-350 (Mar. 1972).

Key words: Archeological materials; bronze; neutron activation analysis; nondestructive analysis; photon activation analysis.

Concentrations of nine major and minor constituents have been determined in samples of two ancient bronze artifacts using neutron and photon activation analysis. The analysis was carried out without chemical separation on 10 mg samples of the material. The results demonstrate the unique capability of nuclear methods for the analysis of small portions of artifacts in archeology.

- 12743.** Seltzer, S. M., Berger, M. J., **Response of NaI detectors to high-energy gamma rays**, *Trans. Amer. Nucl. Soc.* **14**, No. 1, 124-125 (June 1971).

Key words: Detector; electron; gamma ray; Monte Carlo; response function; sodium iodide.

The response of NaI detector to high energy gamma rays has been calculated and compared with experimental results. The calculation takes into account the escape of energy carried by electron, positron and bremsstrahlung.

- 12744.** Sanchez, I. C., DiMarzio, E. A., **Dilute-solution theory of polymer crystal growth. Some thermodynamic and predictive aspects for polyethylene**, *Macromolecules* **4**, 677-687 (Nov.-Dec. 1971).



**Key words:** Activity; chain fold; cilia; equilibrium dissolution temperature; equilibrium melting temperature; free energy of crystallization; lamella thickness; nucleation rate; surface free energy; undercooling.

The kinetic theory of polymer crystallization from dilute solution is applied to the system polyethylene-xylylene. Prerequisite free energy driving forces are derived for crystallization from solution. These naturally depend on bulk thermodynamic properties and three thermodynamic potentials are derived depending on what melt and crystalline properties are assumed. The commonly used  $\Delta H\Delta T/T_m^0$  expression is shown to be an upper bound for all materials and a more accurate expression descriptive of polyethylene is used in the actual calculations. Growth rate and lamella thickness are computed as functions of undercooling, concentration, and molecular weight. It is found that the growth rate varies roughly as concentration raised to a power, the value of the power being a function of both molecular weight and temperature. The isothermal lamella thickness increases only slightly with decreasing molecular weight and is even less dependent on concentration. The isothermal growth rate as a function of molecular weight exhibits a broad maximum. An analysis of the temperature dependence of the growth rate is made in terms of classical nucleation theory using calculations of the present theory as data points. This leads to the concept of an apparent  $\sigma\sigma_e$  which is seen to vary as a function of molecular weight. The theory makes definitive, as yet unverified, predictions which can be tested experimentally.

**12745.** Garvin, D., Evans, W. H., Duncan, B. C., **Some information processing techniques for the small, semi-automated, scientifically-oriented data center**, (Proc. Forum on the Management of Information Analysis Centers, National Bureau of Standards, Gaithersburg, Md., May 17-19, 1971), Chapter in *The Management of Information Analysis Centers*, W. A. Smith, ed., 72-1, 40-57 (Sponsored by The COSAT1 Panel Information Analysis Centers, U.S. Atomic Energy Commission, Oak Ridge, Tenn., Publ., Jan. 1972).

**Key words:** Chemistry; codes for information interchange; editing; information analysis centers; information processing; information retrieval; text handling.

Solutions are presented for several of the problems encountered in handling scientific text in machine-readable form in small data centers. The problems discussed are the selection of an adequate character set for representation of scientific text, the essential and useful features of editing routines, and batch-mode information retrieval.

**12746.** Bridges, J. M., Richter, J., **Arc measurements of Fe I oscillator strengths with improved accuracy**, *Proc. Xth Int. Conf. on Phenomena in Ionized Gases*, Oxford, England, 1971, p. 384 (Donald Parsons and Company, Ltd., Oxford, England, 1971).

**Key words:** Arc; *f*-values; iron; oscillator strengths; wall-stabilized.

Measurements of relative Fe I *f*-values have been performed with greatly improved accuracy over similar previous measurements. The lines are measured in emission from a wall-stabilized argon arc, containing admixtures of FeCl<sub>3</sub> and hydrogen. Recent modifications of the arc allow better control over the iron density, and lead to improved accuracy in relative intensity measurements as well as in plasma diagnostics required for determination of the arc temperature. Results for some selected lines are given, and the program for further measurements is discussed.

**12747.** Scheer, M. D., Fine, J., **The positive and negative self-surface ionization of tantalum**, Chapter 39 in *The Structure and Chemistry of Solid Surfaces*, G. A. Somorjai, ed., pp. 39-1-39-15 (John Wiley & Sons, Inc., New York, N.Y., 1969).

**Key words:** Electron affinities; self-surface ionization; singly charged positive and negative atomic ions; sublimation energies; tantalum.

The sublimation of atoms, singly charged positive, and negative atomic ions of tantalum has been investigated in the 2000-2600 K temperature range with a specially designed mass spectrometer. It was shown that carbon contamination of the tantalum surface could account for the discrepancies previously reported for the energies of atom sublimation. Measurements made on a carbon-free tantalum surface gave values of  $7.94 \pm 0.09$ ,  $11.18 \pm 0.11$  and  $11.2 \pm 0.5$  eV for the sublimation energies of atoms, positive, and negative ions, respectively. The electron affinity of tantalum was found to be  $0.9 \pm 0.3$  eV. These sublimation processes were shown to be consistent with the assumption of thermal equilibration on the tantalum surface and hence can be described by a generalized form of the Saha-Langmuir equation.

**12748.** Miligan, D. E., Jacox, M. E., **Infrared and ultraviolet spectroscopic studies of free radicals and molecular ions isolated in inert solid matrices**, Paper in *Molecular Spectroscopy: Modern Research*, pp. 259-286 (Academic Press, Inc., New York, N.Y., 1972).

**Key words:** Alkali metal reactions; cage effect; flash photolysis; free radicals; infrared spectrum; matrix isolation; molecular ions; molecular orbitals; photolysis; ultraviolet spectrum.

The principles of the matrix isolation technique are reviewed, and results of experiments leading to the stabilization of free radicals in inert solid matrices in concentration sufficient for direct infrared and ultraviolet spectroscopic observation are surveyed. Emphasis is placed on the correlation of the matrix data with data obtained in gas-phase flash photolysis studies. Conclusions regarding the structure and bonding of these species are compared with the predictions of simple molecular orbital theory. Recent results on the infrared and ultraviolet spectra of the C<sub>2</sub><sup>-</sup>, NO<sub>2</sub><sup>-</sup>, and ClHCl<sup>-</sup> ions isolated in an inert, non-ionic environment are also presented.

**12749.** Moore-Sitterly, C., **Committee 4: Structure of atomic spectra**, (Commission 14, International Astronomical Union Report), *Trans. I.A.U.* **14A**, 133-137 (1970).

**Key words:** Atomic spectra; spectra, atomic; structure, atomic spectra.

The present paper is a review of current work on the general subject of analysis of atomic spectra. It deals briefly with programs that are in progress, vacuum UV spectra, rare-earth spectra and theory. A useful bibliography is included.

**12750.** Swanson, N., Kuyatt, C. E., Cooper, J. W., Krauss, M., **Alternative decay channels of a CO<sup>-</sup> Feshbach resonance**, *Phys. Rev. Lett.* **28**, No. 15, 948-951 (Apr. 10, 1972).

**Key words:** CO; CO<sup>-</sup>; decay channels; energy loss spectra; Feshbach resonance.

By means of on- and off-resonance energy-loss measurements, we have observed the decay of the 10.04-eV resonance in CO to the A<sup>1</sup>II, a<sup>3</sup>II, and a'<sup>3</sup>Σ<sup>+</sup> states. The measurements identify the resonance as a <sup>2</sup>Σ<sup>+</sup> state of CO<sup>-</sup>.

**12751.** Pope, C. I., **A simplified method for determining residual thiosulfate in processed microfilm**, *Photogr. Sci. Eng.* **13**, No. 5, 278-279 (Sept.-Oct. 1969).

**Key words:** Archival record film; hypo testing; microfilm; residual thiosulfate.

In the silver nitrate test for residual thiosulfate in processed film the silver ion reacts quantitatively with thiosulfate to form silver sulfide *in situ*. The excess silver ion is removed by treating the sample in solutions of sodium chloride and sodium thiosulfate followed by washing. The method is simplified by using a solution of ammonium hydroxide and sodium chloride to remove the excess silver ion; no washing is necessary. The new method takes half the time previously required.

- 12752.** Schubauer, G. B., **Early developments in hot-wire anemometry at NBS and a look at some elsewhere**, (Proc. Int. Symp. on Hot-Wire Anemometry, University of Maryland, College Park, Md., Mar. 20-21, 1967), Chapter in *Advances in Hot-Wire Anemometry*, W. L. Melnik and J. R. Weske, eds., pp. 13-24 (July 1968).

Key words: Anemometer; hot-wire; measurement of turbulence; turbulence.

The paper reviews the history of hot-wire anemometer development at NBS as applied to the measurement of turbulence. It makes limited mention of work done elsewhere, mainly to place NBS work in proper perspective. The story begins in the middle 1920's with early attempts to measure turbulence, followed by an account of the work of Dryden and Kuethe, which suddenly advanced the hot-wire anemometer as a useful and productive instrument for turbulence measurement. Work at the Technische Hoogeschool at Delft along similar lines, but coming a little later, is described. This is followed by an account of subsequent development of hot-wire equipment at NBS. Finally, departing from NBS work entirely but furthering the theme, "How It Began," an account is given of the birth of the constant-temperature method.

- 12753.** Smith, M. W., Wiese, W. L., **Graphical presentations of systematic trends of atomic oscillator strengths along isoelectronic sequences and new oscillator strengths derived by interpolation**, *Astrophys. J. Supplement Series* 23, Supplement No. 196, 103-196 (June 1971).

Key words: Atomic oscillator strengths; interpolated data; systematic trends.

Recently detected systematic trends of atomic oscillator strengths along isoelectronic sequences are utilized for the determination of new numerical data and for the evaluation of the reliability of existing material. All well-established systematic trends, which number about 100, are presented graphically. New oscillator strengths are interpolated from the graphs, mainly for the higher ions with wavelengths located principally in the vacuum ultraviolet, and are tabulated with their estimated uncertainties. The graphs are ordered according to isoelectronic sequences and are given with full grids to allow the addition of future data.

- 12754.** Simmons, J. H., Macedo, P. B., **Shear and volume structural relaxation in immiscible oxide melts**, (Proc. Conf. Physics of Non-Crystalline Solids, Sheffield, England, Sept. 1970), Chapter 7 in *Amorphous Materials*, R. W. Douglas and B. Ellis, eds., pp. 69-78 (John Wiley and Sons, London, 1972).

Key words: Critical-point effect; immiscible glasses; longitudinal ultrasonics; phase separation; shear ultrasonics; structural relaxation.

The influence of composition fluctuations on the structural relaxation mechanism above the critical point of a series of immiscible oxide glasses is investigated by shear and longitudinal ultrasonic spectroscopy. The results are analyzed to determine the nature of the interaction between the fluctuations in composition and the viscous flow processes.

- 12755.** Rosasco, G. J., Benoit, C., Weber, A., **Light scattering study of the attenuation and dispersion of hypersound in ammonium bromide**, (Proc. 2d Int. Conf. on Light Scattering in Solids, Paris, France, July 19-23, 1971), Chapter in *Light Scattering in Solids*, M. Balkanski, ed., pp. 483-488 (Flammarion Sciences Publ., Paris, France, 1971).

Key words: Acoustic phonons; ammonium bromide; Brillouin scattering; elastic constants; light scattering; relaxation phenomena.

By means of Brillouin scattering, the attenuation and velocity dispersion of hypersonic acoustic waves have been measured in the disordered, cubic phase of  $\text{NH}_4\text{Br}$ . Shear waves determined by the elastic constant  $C_{44}$  show no dispersion. Longitudinal waves propagating in the (001) plane show velocity dispersion and associated attenuation. The  $L$ -mode data are adequately fit by a single relaxation model for the dispersion and attenuation as a function of frequency at 24 °C. The strength of the relaxation,  $[C(\infty) - C(0)]/C(0)$  for the elastic constant  $C_{11}$  is 2.5%; for  $C_{12}$ , 8.8%; and for  $(C_{11} - C_{12})/2$ , 0.6%. The relaxation time measured in this experiment is  $1.16 \times 10^{-11}$  sec. Data which shows that the dispersion increases as the temperature is lowered toward the order-disorder  $\lambda$ -type transition at 234.5 K is also presented. A model is introduced which qualitatively explains the features of this dispersion.

- 12756.** Berger, M. J., Seltzer, S. M., Eisen, H. A., Silverman, J., **Absorption of electron energy in multi-layer targets**, *Trans. Amer. Nucl. Soc.* 14, No. 1, 887-888 (June 1971).

Key words: Absorbed dose; dosimetry; electrons; gamma rays; inhomogeneous media; interface.

This is a report on calculations of electron depth dose distributions in plane-parallel targets consisting of two or more layers of different materials. The cases treated include irradiations with monoenergetic electron beams (0.125 MeV to 1.0 MeV) and cobalt-60 gamma rays.

- 12757.** Sher, A. H., Keery, W. J., Dyson, H. E., **Improved infrared response measurements in semiconductor nuclear radiation detectors**, *IEEE Trans. Nucl. Sci.* NS-19, No. 1, 341-344 (Feb. 1972).

Key words: Defect level; germanium; impurity levels; infrared response; lithium-drifted diodes; semiconductors.

An infrared response technique has been developed which has been shown to yield more detailed spectra than previous techniques and which can be used to identify more specifically energy levels arising from unwanted impurities and defects in semiconductor diodes used as nuclear radiation detectors. The presence of known impurities in germanium detectors, both lithium-compensated and high purity (uncompensated), has been confirmed using this technique. Such impurities include copper, gold, and iron. Features in the spectra associated with crystalline defects have also been identified.

- 12758.** Sher, A. H., Keery, W. J., **Improved infrared-response technique for determining impurity and defect levels in semiconductors**, *Appl. Phys. Lett.* 20, No. 3, 120-122 (Feb. 1, 1972).

Key words: Defect level; germanium; impurity levels; infrared response; lithium-drifted diodes; semiconductors; silicon.

The response of reverse-biased germanium diodes to monochromatic infrared radiation has been studied. Specimens included those fabricated from crystals doped with either copper or gold, or subjected to heat treatment. Preliminary results are reported that show the technique to be useful for identifying such impurities or defects in both lithium-compensated and high purity germanium specimens.



**12759.** Stephenson, N. C., Roth, R. S., **Structural systematics in the binary system  $\text{Ta}_2\text{O}_5$  -  $\text{WO}_3$ . V. The structure of the low-temperature form of tantalum oxide  $L\text{-Ta}_2\text{O}_5$ , *Acta Cryst. B27*, 1037-1044 (1971).**

**Key words:** Crystal structure; low temperature form of  $\text{Ta}_2\text{O}_5$ ; system  $\text{Ta}_2\text{O}_5\text{-WO}_3$ .

The orthogonal unit cell of the compound  $L\text{-Ta}_2\text{O}_5$  has dimensions  $a = 6.198$ ,  $b = 40.29$ ,  $c = 3.888$  Å and contains 11 formula units. The structure was solved in projection from the Patterson function and refined to a conventional  $R$  value of 0.088 using full-matrix least-squares methods. The metal atoms are arranged in sheets and are surrounded by oxygen atoms which form either distorted octahedral or pentagonal bipyramidal coordination polyhedra. The structure contains, on the average, three distortion planes per unit cell. These are statistically distributed over four sites, thereby giving the average unit cell a higher symmetry than the real unit cell. The thermal equilibration of the compound, involving detectable structural changes, is discussed in terms of the migration of distortion planes.

**12760.** Stephenson, N. C., Roth, R. S., **Structural systematics in the binary system  $\text{Ta}_2\text{O}_5\text{-WO}_3$ . IV. The structure of  $\text{Ta}_{38}\text{WO}_{98}$ , *Acta Cryst. B27*, 1031-1036 (1971).**

**Key words:** Crystal structure; system  $\text{Ta}_2\text{O}_5\text{-WO}_3$ ;  $\text{Ta}_{38}\text{WO}_{98}$ .

The structure of the composition  $\text{Ta}_{38}\text{WO}_{98}$  is described in terms of a 19  $\text{UO}_3$ -type subcell unit containing 38 metal atoms and 95.5 oxygen atoms. The orthogonal unit cell has dimensions  $a = 6.188$ ,  $b = 69.57$ ,  $c = 3.880$  Å and the structure was solved in projection from the Patterson function utilizing photographically recorded data. Atomic positional and thermal parameters were refined by least-squares methods to a conventional  $R$  value of 0.118. The composition requires that the unit cell of the equilibrated compound be 429  $\text{UO}_3$ -type subcells. As a result, the description of the structure in terms of an average 19  $\text{UO}_3$ -type subcell unit introduces a splitting of certain atomic peaks. These effects are discussed.

**12761.** Stephenson, N. C., Roth, R. S., **Structural systematics in the binary system  $\text{Ta}_2\text{O}_5\text{-WO}_3$ . III. The structure of  $45\text{Ta}_2\text{O}_5 \cdot \text{Al}_2\text{O}_3 \cdot 4\text{WO}_3$ , *Acta Cryst. B27*, 1025-1031 (1971).**

**Key words:** Crystal structure; system  $\text{Ta}_2\text{O}_5\text{-WO}_3$ ;  $45\text{Ta}_2\text{O}_5 \cdot \text{Al}_2\text{O}_3 \cdot 4\text{WO}_3$ .

The composition  $45\text{Ta}_2\text{O}_5 \cdot \text{Al}_2\text{O}_3 \cdot 4\text{WO}_3$  has an orthogonal unit cell with dimensions  $a = 6.182$ ,  $b = 29.200$  and  $c = 3.876$  Å. This unit cell contains one sixth of a formula unit and differs from  $\text{Ta}_{30}\text{W}_2\text{O}_{81}$  in that it contains a whole number of atoms. The metal atoms are surrounded by either an octahedron or pentagonal bipyramid of oxygen atoms and distortions occur in the shapes of these polyhedra depending on their positions in the unit cell. Metal atoms lie in slightly puckered sheets parallel to (001) and the space group, selected after refinement in a number of plane groups and space groups, is  $P2_1$ . Atomic parameter interactions are shown to be minimized by the use of extensive three-dimensional data. However the interdependence of parameters is determined mainly by the model that is being refined, and the use of the maximum amount of data serves only to minimize rather than remove this intractability.

**12762.** Stephenson, N. C., Roth, R. S., **Structural systematics in the binary system  $\text{Ta}_2\text{O}_5\text{-WO}_3$ . II. The structure of  $\text{Ta}_{30}\text{W}_2\text{O}_{81}$ , *Acta Cryst. B27*, 1018-1024 (1971).**

**Key words:** Crystal structure; system  $\text{Ta}_2\text{O}_5\text{-WO}_3$ ;  $\text{Ta}_{30}\text{W}_2\text{O}_{81}$ .

The structure of the compound  $\text{Ta}_{30}\text{W}_2\text{O}_{81}$  has been determined in projection using single-crystal diffractometer x-ray

data. The orthogonal unit cell has dimensions  $a = 6.172$ ,  $b = 29.226$ ,  $c = 3.850$  Å and contains, on the average, one half of a formula unit. The structure of this unit cell represents the superposition of two structural blocks  $\text{M}_{16}\text{O}_{40}$  and  $\text{M}_{16}\text{O}_{42}$  (where M is a metal atom), which occur in the ratio 3:1. In both structural blocks the metal atoms are arranged in sheets and are surrounded by oxygen atoms forming either distorted octahedral or pentagonal bipyramidal coordination polyhedra. The difference in structure between the two blocks is that in  $\text{M}_{16}\text{O}_{40}$  some metal atoms reduce their coordination numbers to minimize packing distortions. The resultant distortion planes are distributed so that three occur every two unit cell. The asymmetric structural unit was refined in two plane groups,  $pm$  and  $pg$ , using full-matrix least-squares methods. The final  $R$  value is 0.077 and  $pm$  was chosen as the correct plane group on the basis of noncrystallographic considerations.

**12763.** Stephenson, N. C., Roth, R. S., **Structural systematics in the binary system  $\text{Ta}_2\text{O}_5\text{-WO}_3$ . I. The structure of  $\text{Ta}_{22}\text{W}_4\text{O}_{67}$ , *Acta Cryst. B27*, 1010-1017 (1971).**

**Key words:** Crystal structure; system  $\text{Ta}_{22}\text{O}_5\text{-WO}_3$ ;  $\text{Ta}_{22}\text{W}_4\text{O}_{67}$ .

The orthorhombic unit cell of the compound  $\text{Ta}_{22}\text{W}_4\text{O}_{67}$  has dimensions  $a = 6.136$ ,  $b = 47.40$ ,  $c = 3.84$  Å and, on the average, contains one formula unit. The structure was solved in projection from the Patterson function and refined to a conventional  $R$  value of 0.089 using full-matrix least-squares methods. The metal atoms lie in sheets which are separated by  $c = 3.84$  Å. Within each sheet these atoms have a close-packed hexagonal arrangement. Oxygen atoms complete a coordination polyhedron around each metal atom in the form of either a distorted pentagonal bipyramid or octahedron. These polyhedra are joined by edge-sharing within the (001) planes. Extension of the structure along [001] occurs by corner-sharing. The structure differs from one having  $C$ -centered orthorhombic symmetry only in certain areas where metal atoms have reduced coordination numbers. These metal atoms lie in sheets parallel to (010) and the "distortion planes" minimize the anionic packing distortions that would otherwise arise. In this structure there is, on the average, one distortion plane per unit cell.

**12764.** Eisenhauer, C., Chilton, A. B., **Angular distribution of scattered gamma rays from a fan source, *Trans. Amer. Nucl. Soc.* 14, No. 1, 402-403 (June 1971).**

**Key words:** Angular distributions; civil defense; fallout; gamma radiation; Monte Carlo; structure shielding.

The angular distribution of exposure flux due to scattered photons emerging from the wall was calculated by the Monte Carlo method, using the exponential transform technique. Calculations were made for a source energy of 1.25 MeV, concrete thicknesses of 0.5, 1, 1.5, 2, 3, 4, 5, and 6 mean free paths. In order to allow comparison to be made with the OCD Standard Method for Fallout Gamma Radiation Shielding Analysis, the angular distribution of scattered radiation emerging from the wall was tabulated in terms of a polar angle  $\theta$  measured relative to the vertical direction and an azimuthal angle  $\phi$  measured relative to the vertical plane perpendicular to the wall. The angular distribution was grouped into 10 intervals of the polar angle and 6 intervals of the azimuthal angle. A total of 24,000 histories were followed down to a cut-off energy of .02 MeV.

**12765.** Sher, A. H., Liu, Y. M., Keery, W. J., **Infrared response measurements on radiation-damaged Si(Li) detectors, *IEEE Trans. Nucl. Sci.* NS-19, No. 3, 312-317 (1972).**

**Key words:** Defect levels; impurity levels; infrared response; lithium-drifted radiation detectors; semiconductors; silicon.

The improved infrared response (IRR) technique has been to qualitatively compare radiation effects on Si(Li) detectors with energy levels reported for silicon in the literature. Measurements have been made on five commercial silicon detectors and one fabricated in-house, both before and after irradiation with fast neutrons, 1.9-MeV protons, and 1.6-MeV electrons. Effects dependent upon the extent of radiation damage have been observed.

It seems likely that the photo-EMF, or photovoltage effect, is the basic mechanism for the observation of IRR in *p-i-n* diodes with a wide *i*-region. Experimental characteristics of the IRR measurement are in agreement with those of the photovoltage effect.

**12766.** Meinke, W. W., *Some comments on activation analysis, Proc. 2d Inter-American Conference on Radiochemistry, Mexico City, Mexico, Apr. 22-25, 1968*, pp. 54-60 (Published by Secretaría General de la Organización de Estados Americanos, Washington, D.C., 1971).

Key words: Activation analysis; neutron activation; trace analysis; trace characterization.

An overview of the current status of Activation Analysis is given with special note made of the use of neutrons other than reactor-produced neutrons and to the use of separation procedures including group separations. The relation of activation analysis to other methods of analysis is discussed with particular emphasis on the adeptness of the method to handle large numbers of samples for certain elements which are amenable to this method. Activation analysis is inherently an accurate method and its use for trace analysis should join forces with other trace analysis competences to permit a much broader perspective to be applied to the trace analysis problems. The nuclear reactor center with its capability for activation analysis as one facet of general trace competence is a logical focal point for the development of characterization centers to meet the needs in a diverse number of scientific endeavours.

**12767.** Smith, C. N., *Limit of error calculations used in integrated safeguards experiment, Proc. 12th Annual Meeting of the Institute of Nuclear Materials Management, Palm Beach Shores, Fla., June 28-July 1, 1971*, 1, 193-207 (June 1971).

Key words: Integrated Safeguards Experiment; limit of error calculations; nondestructive assay techniques; safeguards.

The Integrated Safeguards Experiment sponsored by the Atomic Energy Commission relied heavily on nondestructive assay techniques to attain a measured material balance on the mixed oxide fabrication process. This paper describes the calculations involved in determining the limit of error values for material measurements using calorimetry and neutron coincidence counting as well as conventional chemical assay methods.

**12768.** Geist, J., Kendall, J. M., Sr., *Circumsolar radiation and the international pyrheliometric scale, Appl. Opt.* **11**, No. 6, 1437-1439 (June 1972).

Key words: Circumsolar radiation; Eppley Angstrom pyrheliometer; international pyrheliometric scale; Primary Absolute Cavity Radiometer.

The responsivity as a function of angle is calculated for Primary Absolute Cavity Radiometers (PACRAD) with 2.45 and 3.32° angular field of view limiting apertures, and for a simplified model of the Eppley Angstrom (E-A) pyrheliometer. From this data, the response of the three instruments to various mathematical models of circumsolar radiation is calculated, and compared

with experimental data obtained during simultaneous measurements of solar irradiance with the three radiometers. The conclusion is that the difference between the values of solar irradiance measured with the 2.45° PACRAD and with the E-A pyrheliometer is not due to circumsolar radiation.

**12769.** Rasberry, S. D., *Application of computers in electron probe and x-ray fluorescence analysis*, (Proc. 20th Annual Conf. on Applications of X-Ray Analysis, Denver, Colo., Aug. 11-13, 1971), Chapter in *Advances in X-Ray Analysis*, K. F. J. Heinrich, ed., 15, 56-69 (Plenum Press, Inc., New York, N.Y., 1972).

Key words: Automatic data acquisition; computer automation of laboratory equipment; computer controlled electron probe; computer controlled x-ray analyzers; electron probe automation.

This paper is a review of automation of electron microprobe and x-ray fluorescence instrumentation. Such a review seems timely because of the great increase in the application of computer systems in this field over the past decade. Some of these applications have been conceived to meet true technological needs while in other cases they have been undertaken to "keep up with the Joneses." I would like to show not only what automated systems are now feasible but also when and how they should be employed. The "when" and "how" of automation are largely dependent upon the application being considered; in this study, x-ray applications have been divided into the following classes: (1) on-stream process-control, (2) off-line quality assurance, (3) routine service laboratory, (4) general-purpose analytical laboratory. Several phases are present in these classes, including: specimen preparation and loading, measurement, data acquisition and transfer, data processing and display, and finally, archival data storage. Various workers have undertaken the automation of all these operations in one or the other of the classes of applications; from a review of their work and by examining details of each operation within the framework of a given application, we can now draw conclusions on the extent of desirable automation.

**12770.** Sugar, J., Kaufman, V., *Fourth spectrum of lutetium, J. Opt. Soc. Amer.* **62**, No. 4, 562-570 (Apr. 1972).

Key words: Lutetium; spectra; theory.

Spectra of lutetium obtained with a sliding spark were photographed in the wavelength range 400-3200 Å. Wavelengths of 246 lines, comprising all lines identified as Lu IV appearing in the spark at 50-A peak current, are given. Fifty-seven energy levels were deduced from these lines, including nearly all levels of the  $4f^{13}(5d, 6s, 6p, 6d, \text{ and } 7s)$  configurations and their connection to the  $4f^{14}^1S_0$  ground state. An ionization energy of  $364\,500 \pm 200$  cm<sup>-1</sup> was derived. The energy levels are interpreted by means of a theoretical analysis utilizing fitted radial parameters. With these results, trends of Slater and spin-orbit parameters and configuration energy differences for fourth spectra of the rare earths are found. The fundamental energy differences between lowest levels of the  $4f^n$  and  $4f^{n-1}5d$  configurations for the fourth and fifth spectra are deduced.

**12771.** Schaffer, R., *Documentation interest of the National Bureau of Standards and collaborating groups for communication of laboratory results in clinical analysis*, (Proc. Conf. Clinically Oriented Documentation of Laboratory Data, Buffalo, N.Y., May 10-12, 1971), Chapter in *Clinically Oriented Documentation of Laboratory Data*, E. R. Gabrieli, ed., pp. 419-424 (Academic Press, Inc., New York and London, 1972).

Key words: Clinical analysis; referee methods for clinical analysis; standard reference materials.



The National Bureau of Standards is actively at work to help clinical laboratories obtain analyses at the level of accuracy that they require and to secure inter-laboratory comparability of results. For achieving these objectives, the Bureau's principal effort has been the certification of Standard Reference Materials for the clinical laboratory. Secondly, a joint program has begun between clinical chemists and NBS for developing referee methods for clinical analysis (methods whose accuracy is known).

**12772.** Schaffer, R., *Isotopic methods*, Paper in *The Carbohydrates, Chemistry and Biochemistry, Second Edition*, W. Pigman and D. Horton, eds., **11B**, 765-776 (Academic Press, Inc., New York and London, 1970).

Key words: Isotope-dilution analysis; isotopic distribution; kinetic isotope effects; labeled carbohydrates.

Isotopically labeled carbohydrates are considered for use as quantitative analytical reagents and for tracing the course of the isotopic portion of a labeled carbohydrate through complex reactions.

**12773.** Shafer, M. R., *Discussion of ASME paper 64-WA/FM-1, density effect and Reynolds number effect on gas turbine flowmeters* by W. F. Z. Lee and H. J. Evans, *J. Basic Eng. Trans. ASME, Series D*, **87**, No. 4, 1052-1053 (Dec. 1965).

Key words: Flowmeters; gas turbine flowmeters; Reynolds number effect on gas turbine flowmeters.

In this discussion of the paper "Density Effect and Reynolds Number Effect on Turbine Meters" by W. F. Z. Lee and H. J. Evans a procedure is suggested for constructing a chart from which the performance of a turbine meter can be predicted when metering any fluid provided compressibility is insignificant. It is believed this suggested procedure may have advantages in some applications over other procedures described in the paper.

**12774.** Forman, R. A., Piermarini, G. J., Barnett, J. D., Block, S., *Pressure measurement made by the utilization of ruby sharp-line luminescence*, *Science* **176**, 284-285 (Apr. 21, 1972).

Key words: Calibration; diamond cell; high-pressure; luminescence.

A rapid, convenient technique for precision pressure measurement in the diamond-anvil high-pressure cell, which makes use of the sharp-line (*R*-line) luminescence of ruby, has been developed. The observed shift is  $-0.77 \pm 0.03$  reciprocal centimeters per kilobar for  $R_1$  and  $-0.84 \pm 0.03$  reciprocal centimeters per kilobar for  $R_2$  to lower energy and is approximately linear in the range studied (to 22 kilobars). Line-broadening has been observed in some instances and has been tentatively identified with nonhydrostatic conditions surrounding the ruby sample.

**12775.** Linsky, J. L., *A proof of the relation between reflectivity and emissivity in an isothermal scattering and absorptive atmosphere*, *J. Quant. Spectrosc. Radiat. Trans.* **12**, No. 5, 777-781 (May 1972).

Key words: Emissivity; planetary atmospheres; reflectivity; spectral line scattering.

A simple relation between directional emissivity and directional hemispherical reflectivity is proven for an isothermal coherent scattering and absorptive atmosphere and also for the case of complete redistribution in a line.

**12776.** Roberts, J. R., Voigt, P. A., Nagy, J. J., *Continuous emission from hydrogen plasmas. I. The theoretical hydrogen emission coefficients*, *Proc. 9th Int. Conf. Phenomena in Ionized Gases, Bucharest, Romania, Sept. 1-6, 1969*, p. 595 (Editura

Academiei Republicii Socialiste Romania, Bucharest, Romania, 1969).

Key words: Continuum; emission coefficients; emission intensity; hydrogen.

Extensive calculations of the continuous hydrogen emission coefficient for a temperature range from 7,000 to 16,000 K and a wavelength range from 1,500 to 15,000 Å have been carried out. The four major reasons for this new calculation are: (a) some of the most recent calculations differ by at least 25 percent in certain spectral regions from these new calculations; (b) a high intensity wall-stabilized hydrogen arc is now available which would allow spectral radiance calibration by means of the accurately calculable hydrogen emission coefficient into the vacuum ultraviolet region and portions of the visible and infrared spectral regions; (c) the contribution of the far wings of Stark broadened hydrogen lines as an addition to this continuum is usually neglected, but will be considered here in detail; and (d) newly available absorption coefficients for  $H^-$  and  $H_2^+$ .

**12777.** Coxon, B., *Conformational analysis via nuclear magnetic resonance spectroscopy*, Article 93 in *Methods in Carbohydrate Chemistry*, R. L. Whistler and J. N. BeMiller, eds., **VI**, 513-539 (Academic Press, Inc., New York, N.Y., 1972).

Key words: Conformational analysis; iterative analysis; long-range coupling constants; n.m.r. spectroscopy; nuclear Overhauser effects; spin-spin coupling constants; variable temperature studies.

Instrumentation for conformational analysis of carbohydrates by n.m.r. spectroscopy is described, together with the preparation of suitable solutions. Spectral assignments may be confirmed by (a) solvent shifts, (b) exchange processes, (c) isotopic substitution, (d) effects of temperature, and (e) double-resonance techniques. Iterative analysis of spectra and interpretation of spin-spin coupling constants over two to five bonds are discussed. The study of conformational equilibria by means of variable-temperature techniques and nuclear Overhauser effects is described. An indication of the potential values of the magnetic resonance of nuclei other than protons is given.

**12778.** Perls, T. A., Stern, J., *Motion*, Chapter 3 in *ISA Transducer Compendium, Second Edition*, Part II, 105-111 (IFI/Plenum, New York, N.Y., June 1970).

Key words: Acceleration transducers; displacement transducers; jerk transducers; measurement of motion; motion transducers; transducer compendium; velocity transducers; vibration transducers.

This introduction to the chapter on motion transducers of the *Second Edition* of the *ISA Transducer Compendium* discusses the various motion measurands covered by the chapter, the principles used for their transduction to electrical signals, and various considerations that enter into the choice of a transducer for specific application.

**12779.** Yokel, F. Y., Somes, N. F., *Performance criteria for tall buildings*, (Proc. 5th CIB Congress, Paris-Versailles, France, June 1971), Chapter in *Research Into Practice, The Challenge of Application 1*, 587-592 (June 1971).

Key words: Building; performance criteria; performance evaluation; structure; tall buildings; user requirements.

The introduction of performance criteria would help to overcome some of the difficulties presently encountered in the design and evaluation of innovative concepts. Performance criteria must be derived from user requirements. The various levels at which performance can be defined result in a hierarchy of performance criteria. The level at which performance should be defined varies for various applications.

An example is presented of performance criteria for structural attributes of buildings and the relationship between these criteria and limit states in structural design.

Recently the Building Research Division of the Institute for Applied Technology, National Bureau of Standards, developed guide criteria for the design and evaluation of innovative housing systems. These criteria are now applied to design, develop, evaluate and certify industrialized housing systems.

Various problems associated with performance evaluation and performance testing are discussed and an example is presented from a structural performance evaluation of a building system that was carried out by the Building Research Division.

**12780.** Stiehler, R. D., Letter to the Editor, *Modern Plastics* **49**, No. 5, 8 (May 1972).

Key words: Specific strength; specific Young's modulus; units of measurement.

Letter to the Editor of *Modern Plastics* correcting the use of the unit "inch" for specific strength and specific Young's modulus.

**12781.** Smith, C. N., X-ray standards for law enforcement, *The Police Chief*, p. 46 (International Association of Chiefs of Police, Gaithersburg, Md., May 1972).

Key words: Law enforcement; voluntary standards; x ray.

Voluntary performance standards for x-ray systems applicable to law enforcement activities are being developed by the Applied Radiation Division of the National Bureau of Standards. The article describes the types of objects subject to x-ray surveillance, the various applications for x-ray systems, and the basic considerations in the formulation of the standards.

**12782.** Liu, Y. M., Coleman, J. A., Radiation damage effects by electrons, protons, and neutrons in Si(Li) detectors, *IEEE Trans. Nucl. Sci.* NS-19, No. 3, 346-352 (1972).

Key words: Electrons; lithium-drifted silicon detector; neutrons; protons; radiation damage; radiation effects; silicon.

The degradation of performance of lithium-compensated silicon nuclear particle detectors induced by irradiation at room temperature with 0.6-MeV and 1.5-MeV electrons, 1.9-MeV protons, and "fast" neutrons from a plutonium-beryllium [Pu-Be] source has been investigated. In general with increasing fluence, the irradiations produced an increase of detector leakage current, noise, capacitance, and a degradation in the performance of the detector as a charged-particle energy spectrometer. Following the irradiations, annealing effects were observed when the detectors were reverse-biased at their recommended operating voltages. Upon removal of bias, a continuous degradation of detector performance characteristics occurred. Detectors which had been damaged by electrons and protons exhibited a stabilization in their characteristics within two weeks after irradiation, whereas detectors damaged by neutrons had a continuous degradation of performance over a period of several months.

**12783.** Radebaugh, R., Siegwarth, J. D., Numerical analysis of continuous and discrete heat exchangers for dilution refrigerators, (Proc. Comm. I, Conf. on Cryophysics and Cryoengineering, Tokyo, Japan, Sept. 11-12, 1970), *Bull. Inst. Int. Froid, Annexe 1970-2*, pp. 57-62 (Int. Inst. of Refrigeration, Paris, France, 1970).

Key words: Cryogenics; dilution refrigerator; heat exchangers; helium-3; helium-4; liquid helium; mixtures.

The design of heat exchangers for dilution refrigerators has proceeded until now with little quantitative information concern-

ing the behavior of the heat exchanger system. In this paper we present results of a numerical analysis on the behavior of both discrete and continuous heat exchangers. Thermal conduction in both the dilute and concentrated streams is taken into account and this requires the solution of two simultaneous second order differential equations for each heat exchanger to determine the temperature distribution. In the case of the discrete heat exchangers, which are required for temperatures below about 0.05 K, the relatively high thermal conductivity of the liquids has a very strong effect on the temperature distribution. In fact for typical dimensions, the liquid temperatures are reasonably constant throughout the heat exchanger and most of the temperature change in each stream occurs in the inlet tubes just before entering the heat exchanger. This implies that the impedance can be reduced by using shorter lengths and larger diameters with little sacrifice in the thermal behavior of the heat exchanger. Figures are presented to aid in the selection of heat exchanger sizes optimized for faster equilibrium times and lower temperatures.

**12784.** Clark, A. F., Kropschot, R. H., Low temperature specific heat and thermal expansion of alloys, (Proc. Comm. I, Conf. on Cryophysics and Cryoengineering, Tokyo, Japan, Sept. 11-12, 1970), *Bull. Inst. Int. Froid, Annexe 1970-2*, pp. 249-254 (Int. Inst. of Refrigeration, Paris, France, 1970).

Key words: Aluminum alloys; copper-nickel alloys; cryogenics; specific heat; stainless steel; thermal expansion; titanium alloys.

Grüneisen was the first to show that statistical thermodynamics could be used to relate thermal expansion and specific heat. Using these relations we have calculated the specific heats of several alloy systems of importance in cryogenic design. Specific heats of copper-nickel alloys, austenitic stainless steels, aluminum alloys and titanium alloys have been calculated in the temperature range 4-300 K and comparisons made with the limited amount of experimental data. Results indicate that, to engineering accuracy, the specific heat of an alloy system can be readily predicted over a large temperature range from the experimentally determined thermal expansion.

**12785.** Andrews, J. R., A frequency calibrator for UHF using an avalanche transistor, *QST LVI*, No. 5, 16-18 (May 1972).

Key words: Avalanche transistor; frequency calibration; impulse; picosecond; spectral intensity; UHF; VHF.

Amateurs have long been accustomed to using 100 KHz crystal oscillators as a source of frequency markers for the calibration of their HF receivers. The frequency calibration of VHF and especially UHF narrow-band receivers has not been as easy. This is because the spectral intensity at VHF of the output from ordinary 100 KHz crystal calibrators has rolled-off into the noise level. This article describes a simple frequency calibrator that provides usable 10 KHz markers to beyond the 1296 MHz band. The calibrator uses a transistor operating in the avalanche mode to generate a 14 volt, 420 picosecond ( $10^{-12}$  seconds) wide impulse into a 50 ohm termination.

**12786.** Oser, H. J., Translator and Editor of the book: *Boundary layers of flow and temperature*, by A. Walz, 297 pages (MIT Press, Cambridge, Mass. 1969).

Key words: Airfoil theory; boundary layer; drag; heat transfer; laminar; lift; skin friction; subsonic; supersonic; transition; turbulent.

A translation of the monograph: *Strömungs-und Temperaturgrenschichten* by Alfred Walz. The book describes theory and computation of laminar and turbulent boundary layers without and with heat transfer.



**12787.** Milligan, D. E., Jacox, M. E., **Infrared and ultraviolet spectroscopic studies of molecular ions trapped in inert solid matrices**, *Proc. 19th Annual Conf. on Mass Spectrometry and Allied Topics*, Atlanta, Ga., May 2-7, 1971, pp. 100-104 (American Society for Mass Spectrometry, ASTM Committee E-14 and Naval Research Laboratory, Washington, D.C., 1971).

Key words: Charge transfer; free radical; infrared spectrum; matrix isolation; molecular ion; ultraviolet spectrum; vacuum-ultraviolet photolysis.

Details of experiments in which diatomic and small polyatomic molecular ions have been trapped in solid argon in sufficient concentration for direct infrared and ultraviolet spectroscopic detection are presented. Among the species for which spectroscopic observations are discussed are  $C_2^-$ ,  $NO^-$ ,  $NO_2^-$ ,  $SO_2^-$ ,  $ClHCl^-$ ,  $BrHBr^-$ ,  $CCl_3^+$ ,  $HCCL_2^+$ , and  $HCCL_2^-$ .

**12788.** Horton, W. S., Carson, C. C., **Gas analysis: Determination of gases in metals**, Chapter 103 in *Treatise on Analytical Chemistry*, I. M. Kolthoff and P. J. Elving, eds., **10**, Part 1, Section E, 6017-6144 (John Wiley & Sons, Inc., New York, N.Y., 1972).

Key words: Gases in metals; hot extraction; nitrogen; Kjeldahl; nitrogen; oxygen; vacuum-fusion analysis.

Methods for the determination of oxygen, hydrogen and nitrogen in metals are discussed. General historical and technical information as well as procedural details and assessment of accuracy for some methods are given. Methods include vacuum-fusion, inert gas fusion, hot extraction, Kjeldahl, spectrographic and isotopic as well as others. This is an invited contribution to form a chapter of Kolthoff and Elving's *Treatise on Analytical Chemistry*.

**12789.** Meyerson, M. R., **Ultrahigh-strength materials**, Chapter 19 in *Materials Science and Technology for Design Engineers*, pp. 366-389 (Hayden Book Company, Inc., New York, N.Y., 1972).

Key words: Alloy steels; ausformed steels; cold-drawn steels; dispersion hardened alloys; fiber and whisker reinforced materials; maraging steels; refractory alloys; stainless steels; strengthening mechanisms; superalloys; titanium alloys; tool steels; ultrahigh strength.

This state of art survey is to be a chapter in a book entitled "Materials Science and Technology for Design Engineers." Written for non-metallurgists, it offers a review of the known strengthening mechanisms and describes the characteristics and mechanical properties of current commercial alloys which attain ultrastrength levels at room and elevated temperatures. Included are alloy steels, tool steels, ausformed steels, cold-drawn steels, hardenable stainless steels, precipitation-hardened stainless steels, maraging steels, titanium alloys, superalloys, refractory alloys, dispersion hardened alloys, and fiber and whisker reinforced materials.

**12790.** Hogen, J. T., **An interesting example of Hund's coupling case (c) in  $HgAr^+$** , *J. Mol. Spectrosc.* **42**, 381-384 (1972).

Key words:  $HgAr^+$ ; Hund's case (c);  $\Omega$ -type doubling; rotational levels.

The rotational energy levels of a diatomic molecule in a Hund's case (c)  $\Omega=1/2$  state arising from  $^2D_{5/2}+^1S_0$  separated atoms are shown to be given by an expression of the form  $B[(J+1/2)^2+8+1/2(p/B)(J+1/2)]-D[(J+1/2)^2+8+1/2(p/B)(J+1/2)]^2$ , where the upper and lower sign choices correspond to rotational levels of parity  $(-1)^{J-1/2}$  and  $(-1)^{J+1/2}$ , respectively, and where  $p \cong +6B$ .

**12791.** King, D. A., Madey, T. E., Yates, J. T., Jr., **Interaction of oxygen with polycrystalline tungsten, Part 3. — Electron stimulated desorption**, *J. Chem. Soc. Faraday Trans. 1*, **68**, 1347-1359 (1972).

Key words: Adsorption; chemisorption; desorption; electron stimulated desorption; oxidation; oxygen; tungsten.

This paper is a sequel to a detailed study of the kinetics of adsorption and desorption in the interaction of  $O_2$  with polycrystalline tungsten, in which a number of oxide and O atom states were identified by thermal desorption. In electron stimulated desorption (ESD) studies two states of adsorbed oxygen were distinguished,  $\beta_1$  and  $\beta_2$ ; the former has a high ESD cross section and the latter a low cross section. In this paper an attempt is made to correlate the states observed in the thermal desorption study with these  $\beta_1$  and  $\beta_2$  states. The ESD properties of the  $\beta_1$  state are determined, and the sticking probability for readsorption onto an oxygen-saturated surface depleted of  $\beta_1$  by ESD is determined as a function of the incremental oxygen coverage. The steady state between electronic desorption and readsorption from the gas phase is examined, and isotopic exchange between  $^{16}O$  and  $^{18}O$  in the  $\beta_2$  and  $\beta_1$  states is observed and characterized. The appearance of the  $\beta_1$  state is related in a complex way to the formation of tungsten oxides which can be thermally desorbed in the temperature range 1200-1600 K.

**12792.** Cox, D. M., Smith, S. J., **Absolute measurement of  $2S$  atom production by dissociative excitation of molecular deuterium**, *Phys. Rev. A* **5**, No. 6, 2428-2442 (June 1972).

Key words: Absolute measurement; cross section; deuterium; dissociative excitation; metastable.

We have measured the cross section for production of metastable ( $2S$ ) atoms by the process of dissociative excitation of molecular deuterium by electron impact. The measurement includes the quantitative evaluation of detection efficiency, density, and geometrical factors necessary to establish an absolute scale on a purely experimental basis. The method depends on the application of an rf field at the Lamb-shift frequency (1059 MHz) to quench the metastables at the point of excitation. The radiation induced by the applied field is isotropic so that the absolute cross section depends on a simple solid-angle correction. The cross sections at 23.8 and 39.1 eV are  $2.97 \times 10^{-18}$  and  $3.40 \times 10^{-18}$  cm<sup>2</sup>, respectively, with a probable error estimated to be  $\pm 14\%$ . The energy dependence of the cross section was also measured from threshold to 500 eV.

**12793.** Opal, C. B., Beaty, E. C., **Measurements of large angle inelastic scattering cross sections for electrons on helium**, *J. Phys. B: At. Mol. Phys.* **5**, No. 2, 627-635 (Mar. 1972).

Key words: Cross section measurements; helium; inelastic scattering.

The ratios of the inelastic electron scattering cross section for the  $n=2$  levels of helium to the corresponding elastic scattering cross sections have been measured in a crossed beam apparatus over the 30 to 150° range for incident energies of 82 and 200 eV. In both cases, at angles greater than 40° the ratio of the sum of the inelastic cross sections to the elastic cross section was constant at a few percent, in qualitative agreement with a similar experiment in atomic hydrogen by Williams. The four  $n=2$  states were observed to have markedly different angular dependencies at 82 eV incident energies. Only the  $^1S$  and  $^1P$  states were important at 200 eV; the ratio  $^1S/^1P$  was very nearly 2 at all angles larger than 60°. Within experimental error, over the range of variables studied, the observed cross sections agreed with those predicted by the first Born approximation only for  $^1P$  at angles less than 45° at 82 eV incident energy and for  $^1S$  and  $^1P$  at 30° and 200 eV incident energy.

**12794.** Hidalgo, M. B., Geltman, S., A high energy approximation: III. Helium excitation by electrons, *J. Phys. B: At. Mol. Phys.* **5**, No. 3, 617-626 (Mar. 1972).

Key words: Coulomb-projected Born; electron impact; excitation; helium; high energy; theory.

The cross sections for the direct excitation of the  $2^1S$  and  $2^1P$  states of helium by electron impact are evaluated in a first order approximation in which the interaction between the incident electron and target nucleus is represented by a coulomb wave final state in the  $T$  matrix. The results obtained for the differential cross sections are much greater than those of the Born approximation for large scattering angles, and the present results are in much better agreement with experiment. The present calculation predicts inelastic differential cross sections which have the asymptotic energy dependence of  $E^{-3}$  for all nonzero angles of scattering. The total cross sections converge to the Born values at high energy.

**12795.** Albers, J., Mountain, R. D., Asymptotic form of the pair-correlation function in liquids, *Phys. Rev. A* **5**, No. 6, 2629-2632 (June 1972).

Key words: Density expansion; liquid structure factor; liquid theory; neutron diffraction; pair correlation function; x-ray diffraction.

Recently, several authors have contended that the pair-correlation function for a simple liquid asymptotically goes to zero in a way proportional to the two-particle potential. We critically examine the basis of their assertion and find that the conclusion is unfounded. Existing x-ray and neutron-diffraction data on liquids are inconclusive insofar as the asymptotic form of the pair correlation is concerned. We propose an experiment which may shed some light upon the large- $r$  behavior of this important quantity.

**12796.** Maienthal, E. J., Polarographic analysis at NBS, *Amer. Lab.* **4**, No. 6, 12-21 (June 1972).

Key words: Analyses; cathode ray polarography; environmental analyses; Standard Reference Materials; trace metals.

A number of applications of cathode ray polarography to the analysis of Standard Reference Materials, research materials, and environmental samples at National Bureau of Standards during the period of July 1968 to June 1970 are discussed. High precision comparative methods for the analyses of major constituents, such as copper in the organo-metallic SRM and high sensitivity subtractive polarographic methods for the determination of trace metals in samples such as fish protein concentrate are described.

**12797.** Bay, Z., White, J. A., Frequency dependence of the speed of light in space, *Phys. Rev. D* **5**, No. 4, 796-799 (Feb. 15, 1972).

Key words: Upper limit of frequency dependence; vacuum dispersion; velocity of light.

To characterize the possible dispersion of the velocity of light in space (vacuum) a Cauchy-type formula,  $n^2 = 1 + A/v^2 + Bv^2$ , is used. It is shown that relativity only allows a nonzero  $A$  term, independent of the nature of the waves or a quantization thereof. Recent experimental data provide upper bounds for  $A$  and  $B$ , limiting thereby the dispersion in the microwave, infrared, visible, and ultraviolet regions of the spectrum to less than one part in  $10^{20}$ .

**12798.** Rathbone, D. Z., Jr., Cutting the costs of cooling, *Plant Eng.* **26**, No. 12, 88-90 (June 15, 1972).

Key words: Amps; condenser water; economy; energy input; outside air wet bulb; power savings; refrigeration production; tons.

Experience with refrigeration production at the NBS central chilled water generation facility has demonstrated that economies in electrical consumption can be achieved by a managed reduction of condenser water temperatures. This paper reports the analysis of refrigeration production using the 3000 ton capacity centrifugal refrigeration compressors during two extremes of condenser water temperatures, and relates that production to the input electrical energy requirements. The conclusion, subsequently verified by operation of the plant according to newly developed operating procedures based upon these observed economies, is that real savings in energy, and consequently money, can be realized by continually maintaining the lowest condenser water temperature (within limits set by the compressor manufacturer) that outdoor weather conditions will permit.

**12799.** Pilling, M. J., Bass, A. M., Braun, W., A curve of growth determination of the  $f$ -values for the fourth positive system of CO and the Lyman-Birge-Hopfield system of  $N_2$ , *J. Quant. Spectrosc. Radiat. Trans.* **11**, 1593-1604 (1971).

Key words: Carbon monoxide;  $f$ -value; nitrogen; transition probability.

The curve of growth method has been employed to determine  $f$ -values for the fourth positive system of CO and the magnetic dipole and electric quadrupole components of the Lyman-Birge-Hopfield system of  $N_2$ . The transition moments are, respectively,  $0.83 a_0 e$ ,  $5.9 \times 10^{-11}$  Bohr magnetons and  $2.6 a_0^2 e$ . No significant dependence on  $r$ -centroid was found. The mean value of the ratio of the electric quadrupole to magnetic dipole  $f$ -values was 0.076.

**12800.** Hubbell, J. H., Survey of photon-attenuation-coefficient measurements 10 eV to 100 GeV, *Atomic Data* **3**, No. 3, 241-297 (Nov. 1971).

Key words: Attenuation coefficient; bibliography; cross section; data index; gamma rays; photons; x rays.

A bibliography of 290 references containing measured absolute-value photon total cross-section data above 10 eV is presented, covering the period 1909 to June 1971. An index by element ( $Z=1$  to  $Z=94$ ) and energy range, characterizing experiments according to source, detector, and number of data points, is included. Graphs are presented for 17 elements ( $Z=1$  to  $Z=92$ ) over the energy range 100 eV to 10 MeV comparing some recent attenuation-coefficient tabulations [by the Lawrence Radiation Laboratory (Livermore), National Bureau of Standards, Los Alamos Scientific Laboratory, and others] with the above documented data points.

**12801.** Spiegel, V., Jr., Evaluation of the neutron source absorption correction in a manganous sulfate bath, (Proc. Amer. Nucl. Soc. National Topical Meeting on Neutron Sources and Applications, Augusta, Ga., Apr. 18-21, 1971), Chapter in *Neutron Sources and Applications*, **II**, 1-170-1-171 (1971).

Key words: Manganous sulfate bath; neutron source calibration; neutron source self-absorption.

A computer code has been written and experimentally verified for the correction to the Manganous Bath Technique for thermal neutron self absorption in spherical and cylindrical neutron sources. The correction is generally small for most absolutely calibrated neutron sources, but may be as large as four or five percent for some commercially available sources with large thermal-neutron cross sections. Neutron multiplication in Pu-Be sources may partially or even overcompensate for neutron absorption. The thermal-neutron flux at the source location, the



source dimensions, and the macroscopic fission and absorption cross sections for all materials in the source are required as program input.

**12802.** Smith, J. M., **Automatic data evaluation, manipulation, display, and plotting with SPEED**, *Comput. Graphics* 4, No. 2, 41-53 (Fall 1970).

Key words: Automatic data evaluation; data conversion; data display; data manipulation; data plotting; digital scanning systems.

SPEED is a system of computer programs written for use in processing data which were automatically recorded on paper or magnetic tape in an engineering laboratory. The basic input is a matrix of values; each row representing a particular time, and each column representing a particular instrument's readings. Since SPEED had been kept general in concept, anyone with such a matrix of input can make use of the programs.

SPEED has three primary phases. In the initial phase data are converted from paper tape, the data from a given instrument may be multiplied by a given coefficient, the converted data are printed and also plotted on the printer. The second phase allows the user to form new artificial data which can be expressed in terms of the input data. This is done using vector arithmetic considering the readings of any given instrument as a vector. In this second phase the user may again obtain printer plots of data. The third phase of SPEED generates pen plots on a CalComp plotter as final, publication quality, output.

**12803.** Karp, S. S., Rath, G. J., Wright, G. P., **A simulation model of admission and discharge policies for an intensive care unit**, *Proc. 1970 Summer Computer Simulation Conference, Denver, Colo., June 10-12, 1970*, pp. 1108-1114 (June 1970).

Key words: Administration; health; hospital; managerial applications; model; policies; queuing model; scheduling; simulation; systems.

A computer simulation model of the admission and discharge policies for an Intensive Care Unit (ICU) of a hospital is described. As determined by the policies being simulated, the model simulates the flow of patients within the hospital, especially with regard to their admittance to and discharge from the ICU. These policies are principally based on the state of health of the individual patients. Thus, the effects of various policies may be predicted in order to select a near optimal set of policies for a given hospital. The description of the pertinent features of the associated General Purpose Simulation System (GPSS) program is also presented.

**12804.** Slattery, W. J., **Standards: Information and sources**, *Proc. 2d Annual Plant Engineering and Western Maintenance Conf., Anaheim, Calif., Sept. 23-25, 1969*, pp. 49-57 (American Institute of Plant Engineers, Region 6, Cincinnati, Ohio, 1969).

Key words: Information sources; KWIC Index; plant engineering; product standards; specifications; standardization; standards.

A brief history of standardization is given. Then four categories of sources of standards information are discussed. The standardization services of the National Bureau of Standards are singled out for discussion with special emphasis on the Product Standards and Information Sections of the Bureau's Office of Engineering Standards Services. A suggestion concerning the mutual exchange of information between the American Institute of Plant Engineers and the NBS is included.

**12805.** Paffenbarger, G. C., **Dental cements, direct filling resins. Composite and adhesive restorative materials: A resume**, (Proc.

Engineering Foundation Research Conferences, Engineering in Medicine-Bioceramics, New England College, Henniker, New Hampshire, August 3-7, 1970), *J. Biomed. Mater. Res. Symp.* No. 2, Part 2, 363-393 (John Wiley & Sons, Inc., New York, N.Y., Jan. 1972).

Key words: Adhesive; cements; composites; cyanoacrylates; dental; methacrylate; polyacrylate; polyurethanes; resins; restorative.

This resume concerns experimental and commercial dental cements and restorative and adhesive materials usually containing nonmetallic inorganic components, the biocompatibility of the above with oral tissues, proposed methods of bioevaluation, the oral environment, the nature of the hard tooth tissue, cavity treatment, agents for bonding the restorative material to the tooth, and 112 references.

The cements include those based on (C-1) zinc oxide-eugenol with additives such as zinc acetate, rosin, polymers and most important *o*-ethoxybenzoic acid (EBA); (C-2) metallic oxides-phosphoric acid; (C-3) acid phosphate salts-water; (C-4) aluminosilicate glass-phosphoric acid; (C-5) zinc oxide-polyacrylic acid; (C-6) methyl methacrylate-poly-(methyl methacrylate) with or without inorganic fillers. Direct filling resins (C-6) without filler and composite restorative materials (C-6) with filler are based on acrylic resins or reaction products of acrylic (methacrylates) with other resins. Coupling agents include cyanoacrylates, epoxy-acrylic adducts and polyurethanes. The 10 tables give composition, values for pertinent physical properties or dental requirements. (C-2) Dominates the cements but (C-1) with (EBA) and (C-5) which has some adhesion to hard tooth tissues and stainless steel may displace (C-2). (C-4) Restorative materials are anticariogenic and widely used but are being supplanted by composite restorative materials.

**12806.** Guevara, F. A., McInteer, B. B., Ottesen, D., Hanley, J. M., **A critique of the high-temperature viscosity measurements of Trautz and Zink**, *Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico, Report No. LA-4643-MS*, pp. 1-10 (June 1971).

Key words: Discrepancy; experimental analysis; viscosity.

Because there is a serious discrepancy between modern dilute-gas viscosity measurements and the values established by pioneering workers, the older experiments of Trautz and Zink are examined in detail. On critical evaluation, the following conclusions seem justified. (1) In the Trautz and Zink measurements there is a systematic error common to all gases. (2) This error may be accounted for by assuming an error in the furnace temperature. (3) No other obvious experimental variable is capable of resolving the systematic discrepancy with modern results. (4) Study of the early apparatus and technique shows that such an experimental error is plausible.

**12807.** Klebanoff, P. S., Tidstrom, K. D., **Mechanism by which a two-dimensional roughness element induces boundary-layer transition**, *Phys. Fluids* 15, No. 7, 1173-1188 (July 1972).

Key words: Boundary layer; roughness; two-dimensional; stability; transition.

An experimental investigation of the effect of two-dimensional roughness elements on boundary-layer transition is described. Primary emphasis is given to the nature of disturbances within the recovery zone, i.e., that region in the immediate downstream of the roughness where the mean flow has been distorted by the presence of the roughness. Detailed measurements of mean velocity distributions, of disturbance spectra, and intensity, growth, and decay of disturbances at discrete frequencies were made for a range of unit Reynolds numbers. The measurements

demonstrate that the behavior can best be understood by considering wave-type disturbances, and the basic mechanism by which a two-dimensional roughness element induces earlier transition to turbulent flow is by the destabilizing influence of the flow within the recovery zone. Comparison with the behavior expected from stability theory supports this conclusion.

- 12808.** Greer, W. L., Rubin, R. J., **Quantum theory of heat transport in an isotopically substituted, one-dimensional, harmonic crystal**, *J. Math. Phys.* **13**, No. 3, 379-385 (Mar. 1972).

**Key words:** Harmonic crystal; heat transport; isotopic disorder; Kapitsa resistance; scattering theory in one-dimension; statistical mechanics; thermal conduction; thermal transport; transport coefficient; wave transmission in random media.

We present a quantum mechanical treatment of thermal transport in a one-dimensional isotopically substituted harmonic lattice. This work is an extension of a classical mechanical treatment. We find that the difference between the quantum and classical expressions for the thermal conductivity of a random chain vanishes in the limit  $N \rightarrow \infty$ , where  $N$  is the number of isotopes. Thus, as in the classical treatment, the thermal conductivity diverges as  $N^{1/2}$ . For a periodic diatomic lattice, we derive explicit formulas for the heat current as a function of temperature. At very low temperatures, this quantum mechanical current exhibits Kapitsa behavior.

- 12809.** Jacox, M. E., Milligan, D. E., **Spectrum and structure of the HO<sub>2</sub> free radical**, *J. Mol. Spectrosc.* **42**, No. 3, 495-513 (June 1972).

**Key words:** ClOO; H-atom reaction; HO<sub>2</sub>; H<sub>2</sub>O<sub>2</sub>; infrared spectrum; matrix isolation; normal coordinate analysis; O<sub>3</sub>; ultraviolet spectrum; vacuum-ultraviolet photolysis.

In studies of the vacuum-ultraviolet photolysis of Ar:O<sub>2</sub>:HCl and Ar:O<sub>2</sub>:H<sub>2</sub>O samples at 14 K the free radical HO<sub>2</sub> has been stabilized in considerably greater concentrations than in earlier experiments, in which the mercury-arc photolysis of HBr or of HI had been used to provide a source of H atoms. Appreciable concentrations of H<sub>2</sub>O<sub>2</sub> and O<sub>3</sub> and, in the experiments using HCl as an H-atom source, of HOCl and ClOO were also stabilized. The infrared spectra of the mixed oxygen-isotopic species of DO<sub>2</sub> have been reported for the first time. The data for the four oxygen-isotopic species of HO<sub>2</sub> have been subjected to a normal coordinate analysis, using a four-constant valence-force field, and the calculated DO<sub>2</sub> frequencies have been compared with the observed values. The previous assignment of the 1389-cm<sup>-1</sup> absorption as the OH deformation fundamental and of the 1101-cm<sup>-1</sup> absorption as the oxygen-oxygen stretching fundamental has been definitively established. A satisfactory fit to the observed absorption pattern for the oxygen-isotopic species of DO<sub>2</sub> has been obtained for a valence angle of  $105 \pm 5^\circ$ . The magnitudes of the two stretching force constants of HO<sub>2</sub> suggest that the electronic structure of HO<sub>2</sub> may approach that of O<sub>2</sub><sup>-</sup>, lending some support to the previous identification of an electronic transition of HO<sub>2</sub> near that of O<sub>2</sub><sup>-</sup>.

- 12810.** Levine, J., Hall, J. L., **Design and operation of a methane absorption stabilized laser strainmeter**, *J. Geophys. Res.* **77**, No. 14, 2595-2609 (May 10, 1972).

**Key words:** Interferometer; methane-absorption stabilized; strainmeter.

A unique 30-meter laser strainmeter is described. The system uses a Fabry-Perot geometry and dynamically adjusts the frequency of the illuminating laser to follow a single fringe. The reference length for the system is provided by a second laser whose wavelength is stabilized by a vibration-rotation absorp-

tion line in methane. The system shows excellent sensitivity, wide bandwidth, and essentially no drift. A sample of the earth-tide record obtained with the laser strainmeter and the initial motion observed for the nuclear explosion Boxcar are shown. The instrument should also be useful for observing free oscillations of the earth.

- 12811.** Winogradoff, N. M., Haller, W. K., Hockey, B. J., **Cross-sectional energy distributions in gigawatt laser pulses: Implications and determination**, *Opto-Electron. Lett.* **3**, 145-148 (1971).

**Key words:** Beam uniformity; glass damage; laser induced sputtering; neodymium glass laser.

Cross-sectional beam uniformity is essential for quantitative work on non-linear optical phenomena and in the measurement of the threshold for laser induced damage in glass. A technique of obtaining detailed information on the beam uniformity by using laser induced sputtering on suitable glass surfaces is described.

- 12812.** Spencer, L. V., Woolf, S., **A "forced-reflection"-type of collimator design**, Paper in Chapter on Shielding and Dosimetry, *Trans. Amer. Nucl. Soc.* **14**, No. 1, 887 (June 1971).

**Key words:** Collimators; multiple neutron backscattering; neutron experimental equipment; neutron-neutron scattering; re-entrant holes; straight ducts.

A collimator design concept is discussed, whereby wall-scattered neutrons are attenuated by an arbitrary number of reflections which are made necessary by choice of tapered segments of appropriate length and angle.

- 12813.** Jednačak, J., Hudomalj, M., Pravdić, V., Haller, W., **Electrokinetics of glass surfaces. I. Charge densities at the solid/gas and the solid/liquid interfaces of porous glasses**, *Croat. Chem. Acta* **44**, 149-156 (1972).

**Key words:** Charge; electrokinetics; glass; surface.

An attempt is described to determine the charge densities at different layers of the surfaces of glass. Three different techniques were used: the heat-of-immersion technique, the electron spin resonance hyperfine splitting measurements, and the electrokinetic streaming potential or current technique.

Estimates of the charge densities at the various interfaces show the structure can be subdivided into the high and low charge portions. The heat-of-immersion technique, looks into the actual solid surface: there the charge density is estimated at in excess of  $10^{14}$  unit e-charges per cm<sup>2</sup>. The hyperfine splitting of the <sup>107</sup>Ag ESR spectrum assumed due to the electrostatic field at the site of the localized atom position: a charge density of 0.7 to  $1.3 \times 10^{13}$  is estimated. It is assumed that the Ag atom is localized in the gel-like layer-solution interface. The excess counterion charge in the diffuse part of the double layer in the liquid phase is estimated at 3 to  $7 \times 10^{12}$ . Thus, the high charge density plane is the interface solid-gel layer. The estimates are based on independent models of the interface structure, widely accepted in literature, although not entirely free of arbitrary assumptions.

- 12814.** Kuyatt, C. E., Plummer, E. W., **Field emission deflection energy analyzer**, *Rev. Sci. Instr.* **43**, No. 1, 109-111 (Jan. 1972).

**Key words:** Electrons; energy analyzer; field emission; high resolution.

A Simpson-Kuyatt type spherical deflection energy analyzer has been adapted to a field emission source. A special decelerating lens allows the analyzer to be used over a wide range of electron energies and energy resolutions. For an electron energy of



2000 eV, a resolution of 20 meV has been demonstrated, while better resolution can be obtained for lower energies ( $\sim 10$  meV at 1000 eV). Special techniques and new design features were employed to make the new analyzer compatible with ultrahigh vacuum ( $\sim 10^{-12}$  torr).

**12815.** Liebman, J. F., Comment on the paper "Oxygen monofluoride (OF,  $^2\Pi$ ): Hartree-Fock wavefunction, binding energy, ionization potential, electron affinity, dipole and quadrupole moments, and spectroscopic constants. A comparison of theoretical and experimental results" by P. A. G. O'Hare and A. C. Wahl, *J. Chem. Phys.* **56**, No. 8, 4242-4243 (Apr. 15, 1972).

Key words: Oxygen fluorides; quantum chemistry; spin conservation.

O'Hare and Wahl recently performed highly accurate calculations on the bonding and energetics of  $^2\Pi$  OF,  $^3\Sigma$  OF $^+$  and  $^1\Sigma$  OF $^-$ . They calculate for the reaction  $^1\Sigma$  OF $^- \rightarrow ^3P$  O +  $^1S$  F $^-$  a  $\Delta G_{298}^\circ$  of  $-9.2$  kJ mol $^{-1}$  and hence OF $^-$  is considered only marginally stable. It is argued only spin-allowed processes should be considered giving a  $\Delta G_{298}^\circ$  of nearly 200 kJ mol $^{-1}$ .  $^3\Sigma$  OF $^+$  is calculated to have a  $D_e$  of 300 kJ mol $^{-1}$  and an EA of 1264 kJ mol $^{-1}$ . The logical but failing, synthetic scheme: OF $_2$  + SbF $_5 \rightarrow$  OF $^+$  SbF $_6$  is discussed and the failure explained by spin conservation. One must form the  $^1\Delta$  state of OF $^+$  and the  $^3\Sigma - ^1\Delta$  separation is estimated as 130 kJ mol $^{-1}$ . We may thus conclude OF $^+$  salts are unlikely.

**12816.** Brinckman, F. E., Johannesen, R. B., Handy, L. B., **Pi-bonding effects in organoxytungsten(IV) fluorides**, *J. Fluorine Chem. Short Commun.* **1**, 493-497 (1971/72).

Key words: Chemical shifts; fluorine NMR; organosilanes; organoxytungsten(VI) fluorides, *Pi*-bonding; substituent parameters; synthesis; tungsten hexafluoride.

Preparation of new substituted phenoxytungsten(VI) pentafluorides by treatment of WF $_6$  with corresponding phenoxytrimethylsilanes permits evaluation of *sigma*- and *pi*-bonding characteristics. Application of  $^{19}\text{F}$  NMR parameters obtained for these compounds to well-established correlations thereby yield substituent parameters for the  $-\text{OWF}_5$  group; it is shown that results are consistent with a strong inductive withdrawal effect ( $\sigma_I = +0.9$ ) and a small *pi*-acceptor effect ( $\sigma_R = +0.07$ ). Alternatively, inspection of the  $-\text{WF}_5$  moiety reveals the chemical shift of F *trans* to the ligand, as compared to that for equatorial F, shows a marked dependence on the *pi*-donor properties of the ligand.

**12817.** Becker, D. A., LaFleur, P. D., **Determination of trace quantities of uranium in biological materials by neutron activation analysis using a rapid radiochemical separation**, *Anal. Chem.* **44**, No. 8, 1508-1511 (July 1972).

Key words: Biological materials; neutron activation analysis; rapid radiochemical separation; solvent extraction; trace analysis; uranium.

Neutron activation analysis has been applied to the determination of trace quantities of uranium in biological materials, using the short-lived radioisotope  $^{239}\text{U}$  ( $T_{1/2} = 23.5\text{m}$ ). A solvent extraction technique was developed for the extraction of uranium by the reagent hydrogen bis(2-ethylhexyl) phosphate (HDEHP). The technique developed was found to be applicable also to the analysis of uranium in other materials such as aluminum, copper oxide and zirconium. Extraction efficiencies for uranium using HDEHP are presented for nitric, perchloric, hydrochloric and hydrofluoric acids. The analysis for uranium at levels of  $10^{-6}\text{g}$  to  $10^{-9}\text{g}$  was made in practical samples, and good agreement obtained with other analytical techniques.

**12818.** Leung, P. S., Rush, J. J., Taylor, T. I., **Study of hindered rotation in crystals by neutron transmission measurements: Comparison of calculated and measured scattering cross sections**, *J. Chem. Phys.* **57**, No. 1, 175-182 (July 1, 1972).

Key words: Ammonium salts; cross section; crystals; hindered rotation; methylbenzenes; neutron scattering; torsional vibrations.

Total neutron cross sections have been measured as a function of neutron wavelength ( $\lambda_n = 5 - 11$  Å) and sample temperature for (NH $_4$ ) $_2$ SiF $_6$ , (NH $_4$ ) $_2$ S $_2$ O $_8$ , durene and hexamethylbenzene. The experimental results are compared to previous cross-section data for other ammonium salts and methyl-substituted compounds and are correlated with the rotational freedom of the NH $_4^+$  ions and methyl groups. A relatively simple theoretical procedure is described for calculating total scattering cross sections of hydrogenous crystals using torsional and translational lattice-mode frequencies obtained from neutron or optical spectra. Cross-section variations vs wavelength ( $\Delta\sigma_s/\Delta\lambda$ ) and temperature ( $\Delta\sigma_s/\Delta T$ ) are calculated for a large group of ammonium salts and methyl-substituted organics (including those for which experimental cross sections are presented here) and are directly compared with measured cross section results. In every case the experimental and theoretical results agree within about 10% or less. Thus the previously observed empirical relationship between  $\Delta\sigma_s/\Delta\lambda$  and  $\Delta\sigma_s/\Delta T$  and the rotational and vibrational behavior of ions and molecules in solids is placed on a more quantitative basis. These comparisons reinforce the usefulness of the neutron cross-section method as a supplement to spectroscopic techniques.

**12819.** Prince, E., **Configuration of the water molecule in cupric fluoride dihydrate at 298 K**, *J. Chem. Phys.* **56**, No. 9, 4352-4355 (May 1, 1972).

Key words: Bond angle; diffraction; fluoride; hydrate; hydrogen bond; neutron diffraction; structure refinement; thermal motion; water molecule.

The crystal structure of cupric fluoride dihydrate at 298 K has been redetermined from three-dimensional, single crystal, neutron diffraction data. Least-squares refinement of 163 independent, observed reflections gave a final, weighted *R* index  $R_w = 0.038$ . The H—O—H angle in the water molecule is  $110.6 \pm 0.2^\circ$ , which, in contrast to the value  $115.5 \pm 0.4^\circ$  found in an earlier study, is not significantly different from the tetrahedral angle of  $109.5^\circ$ . Thermal vibration is highly anisotropic, with much larger amplitudes perpendicular to infinite, hydrogen-bonded sheets than parallel to the sheets.

**12820.** Kurylo, M. J., **Absolute rate constants for the addition of O( $^3\text{P}$ ) atoms to propylene**, *Chem. Phys. Lett.* **14**, No. 1, 117-120 (May 1, 1972).

Key words: Hydrogen atoms; propylene; reaction rate; resonance fluorescence.

The rate of addition of oxygen ( $^3\text{P}$ ) atoms to propylene has been investigated by the flash photolysis resonance fluorescence technique. Using O $_2$  as the atom source, the reaction was studied from 201 to 424 K. A linear least squares treatment of the Arrhenius data gave:  $k = (4.17 \pm 0.33) \times 10^{-12} \exp[-(76 \pm 44)/1.987T]$  in units of cm $^3$  molecule $^{-1}$  sec $^{-1}$ .

**12821.** Marchetti, M. A., Krauss, M., Weiss, A. W., **Symmetry-adapted pair correlations in O and O $^-$** , *Phys. Rev. A* **5**, No. 6, 2387-2390 (June 1972).

Key words: Electron affinity; O, O $^-$ ; pair-correlation energy; shell-correlation energy; symmetry-adapted.

A symmetry-adapted pair-correlation approximation has been used to calculate the electron affinity of the oxygen atom. The

calculated electron affinity is 1.47 eV which is in reasonable agreement with experimental values. The present results add to the evidence that the energy difference between similar systems can be calculated with reasonable accuracy using symmetry-adapted pair energies.

**12822.** de Graaf, L. A., Rush, J. J., Flotow, H. E., Rowe, J. M., **Quasielastic thermal neutron scattering by hydrogen in  $\alpha$ -vanadium hydride**, *J. Chem. Phys.* **56**, No. 9, 4574-4581 (May 1, 1972).

**Key words:** Debye-Waller factor; hydrogen diffusion, interstitial site; linewidth; momentum transfer; neutron scattering, quasielastic scattering; vanadium hydride; vibration.

The diffusion process of hydrogen in vanadium has been studied by quasielastic thermal neutron scattering. Neutron linewidths associated with diffusion broadening have been determined at 485 K for  $\text{VH}_{0.198}$  and  $\text{VH}_{0.570}$ . These measurements cover a range of momentum transfers ( $Q$ ) for elastic scattering up to  $4.1 \text{ \AA}^{-1}$ . This is much larger than the momentum transfers obtained in earlier cold-neutron experiments, where no conclusive comparison was possible between data and proposed models involving diffusive jumps between octahedral and tetrahedral sites. The linewidth results for  $\alpha\text{-VH}_{0.57}$  are compared with these models and with an extension developed in the present paper. Although no complete agreement was obtained, this comparison leads to the conclusion that jumps between tetrahedral sites are predominant in the diffusion process. Differences in the linewidth behavior for  $\text{VH}_{0.198}$  and  $\text{VH}_{0.570}$ , and the fact that the measured widths at large  $Q$  increase rapidly with  $Q$  rather than approaching an asymptotic value as predicted by the theory, are discussed. It is suggested that these effects and the large Debye-Waller factors found in the present and previous neutron experiments are connected with the relative magnitudes of diffusion relaxation time and the jump time between sites.

**12823.** Davis, D. D., Huie, R. E., Herron, J. T., Kurylo, M. J., Braun, W., **Absolute rate constants for the reaction of atomic oxygen with ethylene over the temperature range 232-500 K**, *J. Chem. Phys.* **56**, No. 10, 4868-4876 (May 15, 1972).

**Key words:** Absolute rate constants; atomic oxygen; ethylene; gas phase kinetics.

Rate constants for the reaction of atomic oxygen with ethylene were measured over a temperature range of 232-500 K using the flash photolysis-resonance fluorescence technique. The rate constant at room temperature was also determined using a flash photolysis-kinetic absorption spectroscopy system and a discharge-flow system coupled to a mass spectrometer. Within the experimental errors of the three techniques, good agreement was found for the rate constant at 298 K. The bimolecular rate constant was also found invariant to changes in both total pressure and reactant concentration. Over the temperature range of the experiments, the rate data could be fitted by a simple Arrhenius expression of the form,

$$k = 5.42 \pm 0.30 \times 10^{-12} \exp\left[(-1130 \pm 32 \text{ cal mole}^{-1})/RT\right] \text{ cm}^3 \text{ molecule}^{-1} \cdot \text{sec}^{-1}.$$

**12824.** Eby, R. K., Colson, J. P., **Alpha relaxation in polyethylene**, *J. Appl. Phys.* **41**, No. 11, 4313-4316 (Oct. 1970).

**Key words:** Annealing; density; lamella thickness; mechanical; polyethylene; relaxation; solvent; unit cell.

Data are presented to show that a previously reported correlation of the strength of the alpha relaxation in annealed solution-grown crystals of polyethylene with the inverse of lamella thickness is not unique. Nor is a previously reported dependence of relaxation temperature on lamella thickness unique. As the lamella thickness changes with annealing temperature, the unit

cell dimensions, the macroscopic density, and the residual solvent content of the crystals also change. Thus, there are apparent correlations between these parameters and the relaxation strength and temperature. Since it is not obvious which, if any, of these correlations is the fundamental one with regard to the alpha relaxation, some caution must be exerted in interpreting them. As an example of this, data are discussed to suggest that there is at least one other presently unknown parameter of importance to the relaxation.

**12825.** Scheer, M. D., Klein, R., McKinley, J. D., **Halogens adsorbed on molybdenum: their surface lifetimes and desorption kinetics**, *Surface Sci.* **30**, No. 2, 251-262 (Apr. 1972).

**Key words:** Desorption kinetics; halogen surface lifetimes; molybdenum; negative surface ionization.

The surface lifetimes of fluorine, chlorine, bromine and iodine adsorbed on a molybdenum surface have been obtained from measurements of the halide ion desorption flux using the modulated molecular beam technique. Measurements were made at temperatures between 1350 and 1850 K and at surface coverages of less than  $10^{10}$  halogen atoms  $\text{cm}^{-2}$ . The temperature-lifetime data were fitted to an Arrhenius expression from which the binding energies,  $\bar{l}$ , and pre-exponential factors  $\tau^0$ , were obtained:

$$\begin{aligned} \text{F: } \bar{l} &= 4.65 \text{ eV} \quad \text{and} \quad \tau^0 = 3 \times 10^{-16} \text{ s;} \\ \text{Cl: } \bar{l} &= 4.11 \text{ eV} \quad \text{and} \quad \tau^0 = 3 \times 10^{-16} \text{ s;} \\ \text{Br: } \bar{l} &= 3.70 \text{ eV} \quad \text{and} \quad \tau^0 = 2 \times 10^{-15} \text{ s;} \\ \text{I: } \bar{l} &= 3.15 \text{ eV} \quad \text{and} \quad \tau^0 = 1 \times 10^{-11} \text{ s.} \end{aligned}$$

It was concluded that the halogens are adsorbed as strongly bound surface compounds,  $\text{MoX}$  (where X is either F, Cl, Br, or I) from which gaseous ions and neutral atoms desorb at rates consistent with the Saha-Langmuir relationship. From that relationship and the above data, separate binding energies and pre-exponentials were calculated for ion and neutral desorption. The importance of the desorption of  $\text{MoX}$  was assessed.

**12826.** Reader, J., Epstein, G. L., **Analysis of the spectrum of quadruply ionized yttrium ( $\text{Y}^{4+}$ )**, *J. Opt. Soc. Amer.* **62**, No. 5, 619-622 (May 1972).

**Key words:** Spectra; ultraviolet; wavelengths; yttrium.

The  $\text{Y}^{4+}$  spectrum has been observed in a sliding-spark discharge with the NBS 10.7-m normal-incidence vacuum spectrograph. The analysis has yielded all the levels of the  $4p^4 5s$  configuration and nearly all levels of  $4p^4 4d$  that can combine with the  $4p^5 \text{ } ^2P$  ground term. The  $4s^2 4p^4 4d + 4s^2 4p^4 5s + 4s 4p^6$  levels have been theoretically interpreted, including configuration-interaction effects. The  $4s 4p^6 \text{ } ^2S_{1/2}$  level was found to have a 26%  $4s^2 4p^4 d(D)^2 S$  character and the  $4s^2 4p^4 d(D)^2 S_{1/2}$  level a 22%  $4s 4p^6 \text{ } ^2S$  character. The energy parameters determined from a least-squares fit of the observed level values are compared with Hartree-Fock calculations. The ionization energy is estimated to be  $75.0 \pm 0.5 \text{ eV}$ .

**12827.** Barnes, J. D., Fanconi, B. M., **Raman spectroscopy, rotational isomerism, and the "rotator" phase transition in  $n$ -alkanes**, *J. Chem. Phys.* **56**, No. 10, 5190-5192 (May 15, 1972).

**Key words:**  $n$ -alkanes; Raman spectroscopy; rotator phase; rotational isomerism.

Raman spectra of  $n$ -nonadecane in the ordered and rotator phases are compared to that of the liquid phase to determine the amount of rotational isomerism in the rotator phase. It is concluded that there is little or no rotational isomerism in the rotator phase.



**12828.** Okabe, H., Photodissociation of CS<sub>2</sub> in the vacuum ultraviolet; determination of D<sub>0</sub><sup>0</sup>(SC-S), *J. Chem. Phys.* **56**, No. 9, 4381-4384 (May 1, 1972).

Key words: Bond dissociation energy; CS<sub>2</sub>; CSA<sup>1</sup>Π; D<sub>0</sub><sup>0</sup>(SC-S); fluorescence; photodissociation; vacuum ultraviolet.

It has been shown that a major primary photochemical process of CS<sub>2</sub> in the vacuum ultraviolet is the reaction,



in apparent violation of the spin conservation rule. From the threshold energy of incident photons required to produce the fluorescence, CS A<sup>1</sup>Π - X<sup>1</sup>Σ, D<sub>0</sub><sup>0</sup>(SC-S) = 4.463 ± 0.014 eV or 102.9 ± 0.32 kcal/mole has been obtained in excellent agreement with the value derived previously from the photoionization of CS<sub>2</sub>. Other related thermochemical data are derived and are compared with those obtained by various methods. The fluorescence excitation spectrum shows peaks corresponding to Rydberg series I and II, indicating that the above reaction is mainly the result of predissociation from Rydberg states. The fluorescence efficiencies became quite small above incident photon energies corresponding to the first ionization potential of CS<sub>2</sub>. The CS A<sup>1</sup>Π fluorescence spectrum produced by the 1236 Å line photolysis shows vibrational levels populated up to v' = 5. The absorption coefficient of CS<sub>2</sub> has been measured in the region 1200–1400 Å.

**12829.** Camus, P., Sugar, J., Theoretical study and interpretation of the electronic configurations in Tm II. II. Odd excited configurations 4f<sup>12</sup>(5d+6s)6p and 4f<sup>13</sup>7s, *Phys. Scr.* **4**, 263-268 (1971).

Key words: Energy levels; theory; thulium.

The calculation of the energy eigenvalues and the Lande g factors of the configuration 4f<sup>12</sup>(5d+6s)6p taken together has allowed the identification of 175 odd levels with a mean error of 97 cm<sup>-1</sup>. The configuration 4f<sup>12</sup>5d6p is identified at 44 838 cm<sup>-1</sup>. The eigenvectors of f<sup>12</sup>sp and those of f<sup>12</sup>dp for the matrices with J greater than or equal to 5 are given in the \*J<sub>1</sub>J<sub>2</sub> coupling scheme where \*J<sub>1</sub> is an eigenvector of the real core of f<sup>12</sup>. The four levels of the configuration 4f<sup>13</sup>7s are interpreted and the value of the IP of Tm II fitted by interpolation with the neighbouring elements, which is 12.05 volts, is confirmed.

**12830.** Camus, P., Sugar, J., Theoretical study and interpretation of the electronic configurations in Tm II. I. Even configurations 4f<sup>12</sup>(5d+6s)<sup>2</sup>+4f<sup>13</sup>6p, *Phys. Scr.* **4**, 257-261 (1971).

Key words: Energy levels; theory; thulium.

The calculation of the energy eigenvalues and the Lande g factors of the configurations 4f<sup>12</sup>(5d+6s)<sup>2</sup>+4f<sup>13</sup>6p taken together has led to the interpretation of 155 even levels whose energies are predicted with an rms error of 105 cm<sup>-1</sup>. The configuration 4f<sup>12</sup>5d<sup>2</sup> is correlated with 36 experimental levels, among which is the lowest level at 30 508 cm<sup>-1</sup>. Eigenvectors of the subgroup of configurations f<sup>12</sup>ds+f<sup>13</sup>p are given in the J<sub>1</sub>J<sub>2</sub> coupling scheme, which is the closest to the physical coupling.

**12831.** Tsang, W., Comparative rate single-pulse shock tube studies on the thermal decomposition of cyclohexene, 2,2,3-trimethylbutane, isopropyl bromide, and ethylcyclobutane, *Int. J. Chem. Kinet.* **11**, 311-323 (1970).

Key words: Bond energy; cyclohexane; decomposition; gas phase; isopropyl bromide; shock tube; t-butyl radical decyclization; 2,2,3-trimethylbutane.

A check of the data from comparative rate single-pulse shock tube experiments has been carried out through the use of a new

standard reaction, the decyclization reaction of ethylcyclobutane. The rate expressions for cyclohexane and 2,2,3-trimethylbutane have been found to be

$$k(C_6H_{10} \rightarrow 1,3-C_4H_6 + C_2H_4) = 10^{15.3} \exp(-33,690/T) \text{ sec}^{-1}, \\ 950-1100 \text{ K}, 2-6 \text{ atm}$$

$$k(tC_4H_9 \rightarrow iC_3H_7 \rightarrow tC_3H_9 + iC_3H_7)$$

$$= 10^{16.5} \exp(-36,830/T) \text{ sec}^{-1}, 1000-1100 \text{ K}, 2-6 \text{ atm}$$

in excellent agreement with previously published results. Most of the small discrepancy that does exist is apparently due to the differences between the present and earlier (decomposition of isopropyl bromide) "standard" reaction. For the latter process, the present study yields

$$k(iC_3H_7Br \rightarrow C_3H_6 + HBr)$$

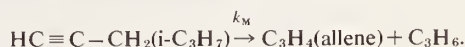
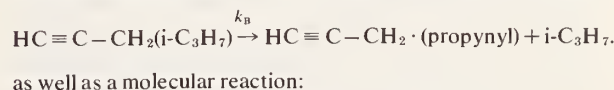
$$\rightarrow 10^{13.73} \exp(-23,970/T) \text{ sec}^{-1}, 800-1000 \text{ K}, 2-6 \text{ atm}$$

These results confirm the correctness of previously published comparative rate single-pulse shock tube experiments. They demonstrate once again that for the decomposition of paraffin hydrocarbons, calculated preexponential factors are at least an order of magnitude higher than the directly measured number and that the accepted value of the heat of formation of t-butyl radicals ΔH<sub>f300</sub>(tC<sub>4</sub>H<sub>9</sub>·) = 29 kJ (6.8 kcal) is at least 10 kJ too low. Finally, attention is called to recent studies on neopentane decomposition in flow and static systems which are in complete agreement with the present conclusions.

**12832.** Tsang, W., Rate and mechanism of thermal decomposition of 4-methyl-1-pentyne in a single-pulse shock tube, *Int. J. Chem. Kinet.* **11**, 23-36 (1970).

Key words: Allene; bond energy; comparative rate; gas phase; heats of formation; kinetics; molecular reaction; propynyl; pyrolysis; single-pulse shock tube; 4-methylpentyne-1.

Dilute mixtures of 4-methyl-1-pentyne have been pyrolyzed in a single-pulse shock tube. The decomposition process involves bond breaking:



The rate parameters are:

$$k_B = 10^{15.56} \exp(-34,940/T) (\text{sec}^{-1})$$

$$k_M = 10^{13.1} \exp(-29,670/T) (\text{sec}^{-1}) \quad 1100 \text{ K}, 1.5-5 \text{ atm}$$

The heat of formation of propynyl radical is thus ΔH<sub>f300</sub> = 338 kJ mol<sup>-1</sup> (80.7 kcal mol<sup>-1</sup>). This leads to a propynyl resonance energy of 40 kJ mol<sup>-1</sup> (9.6 kcal mol<sup>-1</sup>).

**12833.** Ehrlich, M., Response of thermoluminescent dosimeters to 15 MeV electrons and <sup>60</sup>Co gamma rays, *Health Phys.* **18**, 287-289 (1970).

Key words: Absorbed dose; CaF<sub>2</sub>:Dy; dosimeters; LiF; response; thermoluminescence; 15 MeV electrons; <sup>60</sup>Co gamma rays.

Thermoluminescence dosimeters (TLD) were mailed along with Fricke dosimeters to some of the participants in the NBS electron-dosimetry uniformity studies, for irradiation with 15 MeV electrons in a polystyrene block. The electron-irradiated TLD and Fricke dosimeters then were returned to NBS for evaluation along with similar dosimeters exposed at NBS to <sup>60</sup>Co

gamma rays. Three TLD systems were used: LiF TLD-100 plaques, LiF TLD-100 powder in gelatine capsules, and  $\text{CaF}_2\text{:Dy}$  TLD-200 plaques. For the gamma rays, absorbed dose in the TLD material was computed from exposure, and for the electrons, it was computed from the absorbed dose measured in the Fricke dosimeters. Within the limits of experimental precision and the reliability of the computations, the relative TL response per unit absorbed dose in the three systems was found to be the same for  $^{60}\text{Co}$  gamma rays and for 15 MeV electrons.

- 12834.** Wilson, W. K., Hebert, R. L., **Evaluation of the stability of manifold papers**, *Tappi* **55**, No. 7, 1103-1107 (July 1972).

Key words: Aging; alkalinity; burst strength; degradation; differential thermal analysis; durability; manifold papers; loads; pH; reflectance; stability; storage; tear strength; testing.

The relative stabilities of a group of seven manifold papers were determined by accelerated aging in flowing air at 90 °C and 50% relative humidity. One alkaline paper, one neutral-sized paper, and five acid papers were included. Changes during aging were noted by monitoring folding endurance, pH, tearing strength, bursting strength, load elongation, and reflectance. The alkaline paper was very stable, the neutral-sized paper somewhat less stable, and the acid papers could be ranked in stability approximately according to their pH values. The temperature at which a massive decomposition endotherm (differential thermal analysis) occurred also appeared to be a function of pH.

- 12385.** Schaffer, R., **Occurrence, properties, and preparation of naturally occurring monosaccharides (including 6-deoxy sugars)**, Chapter in *The Carbohydrates. Chemistry and Biochemistry*, Second Edition, W. Pigman and D. Horton, Eds., **1A**, 69-111 (Academic Press, Inc., New York, N.Y., 1972).

- 12836.** Young, R., Ward, J., Scire, F., **Observation of metal-vacuum-metal tunneling, field emission, and the transition region**, *Phys. Rev. Lett.* **27**, No. 14, 922-924 (Oct. 4, 1971).

Key words: Field emission; MVM tunneling; surface finish; surface physics; tunneling.

We report what we believe are the first observations of metal-vacuum-metal tunneling. A field emitter is brought close to a metal surface and the current-voltage characteristic is measured in three regions: the Fowler-Nordheim region, the intermediate region, and the metal-vacuum-metal region.

- 12837.** Young, R. D., **Surface microtopography**, *Phys. Today* **24**, No. 11, 42-49 (Nov. 1971).

Key words: Microscope; microtopography; single-crystal surface; surface; surface finish; surface profile.

The growing field of surface science would benefit considerably from measurements of surface microtopography down to the atomic level. A brief review is presented of several instruments used to quantitatively characterize the surface microtopography of metallic surfaces. Techniques are discussed for employing the transmission electron microscope, the scanning electron microscope, the optical interference microscope and an engineering profile measuring instrument to measure surfaces suitable for surface science experiments. In addition a new noncontacting instrument, which is presently under development will be described. It is concluded that several techniques are presently available for detecting single atom steps on single-crystal surfaces.

- 12838.** Berger, M. J., Seltzer, S. M., **Bremsstrahlung in the atmosphere**, *J. Atmos. Terr. Phys.* **34**, 85-108 (1972).

Key words: Aurora; balloon experiments; bremsstrahlung; electrons; energy spectrum; sodium iodide detectors.

Calculations are described pertaining to the emission of bremsstrahlung by electrons in the upper atmosphere and the penetration of this radiation to atmospheric depths of 3-10 g  $\text{cm}^{-2}$  where it can be measured by balloon-borne detectors. The calculations take into account the multiple scattering and slowing down of electrons, and the multiple Compton scattering and photoelectric absorption of bremsstrahlung photons. Numerical data have been generated for electron beams incident onto the atmosphere with energies between 20 keV and 2 MeV, assuming wide-area precipitation and an incident angular distribution isotropic over the downward hemisphere. The results relate the number and energy spectrum of the incident electrons to the bremsstrahlung flux spectrum at balloon heights. The interpretation of some observed bremsstrahlung flux spectra is attempted.

- 12839.** Sugar, J., **Potential-barrier effects in photoabsorption. II. Interpretation of photoabsorption resonances in lanthanide metals at the 4d-electron threshold**, *Phys. Rev. B* **5**, No. 5, 1785-1792 (Mar. 1, 1972).

Key words: Lanthanides; metallic spectrum; photoabsorption.

The resonances in the photoabsorption spectra of the lanthanides near the 4d absorption edge are interpreted as transitions of the type  $4d^{10}4f^N \rightarrow 4d^9 4f^{N+1}$ . Calculations of the  $4d^9 4f^{N+1}$  energy levels and relative *gf* values for these transitions are shown to be in good agreement with the observed absorption spectra. The assumption that the lanthanides occur in trivalent form (with the exception of Eu and Yb) in the metallic solid state is confirmed by these results.

- 12840.** Srinivasan, G. R., Tweer, I., Macedo, P. B., Sarkar, A., Haller, W., **Phase separation in  $\text{SiO}_2\text{-B}_2\text{O}_3\text{-Na}_2\text{O}$  system**, *J. Non-Cryst. Solids* **6**, 221-239 (1971).

Key words: Electron microscopy; immiscible oxide; nucleation and growth; phase decomposition; phase separation; sodium-borosilicate.

Isothermal studies of the phase separation occurring in the  $\text{SiO}_2\text{-B}_2\text{O}_3\text{-Na}_2\text{O}$  system near the center of the miscibility gap are made at three temperatures. Early stage observations of the phase morphology indicate that phase interconnectivity is probably due to nucleation and subsequent intersecting growth of silica-rich particles. It is found also that the extent of interconnectivity is strongly dependent on the volume ratio of the coexisting phases. Evidence is also presented that the glass of present composition is in a two-phase region rather than the three-phase region previously reported. It is also shown that there is very little rotation of the tie-lines between 748 and 650 °C.

- 12841.** Fuller, E. G., **Nuclear reaction theory and the photonuclear giant resonance**, (Proc. 5th Congress of Yugoslavian Mathematicians, Physicists and Astronomers, Skopje, Yugoslavia, Sept. 13-14, 1972), *Physics*, Vol. II, No. 5, 5-10 (Macedonian Society of Mathematicians, Physicists and Astronomers, Skopje, Yugoslavia, 1972).

Key words: Coupled-channel; eigenchannel; giant resonance; photonuclear; reaction theory.

A brief review is given of the continuum theory of nuclear reactions with particular emphasis on the eigenchannel and coupled channel approaches as applied to the photonuclear giant resonance. Comparison of the theoretical results with experimental data indicates that at best the existing theories can describe only the gross features of the giant resonance. The experimental data seem to indicate the existence of large coherence effects in the giant resonance region.



**12842.** Goldberg, R. N., Frank, H. S., **Liquid junction potentials and single-ion activities by computer simulation. I. The concentration cell with transference**, *J. Phys. Chem.* **76**, No. 12, 1758-1762 (1972).

Key words: Computer simulation; electrochemistry; ionic activities; liquid junction potentials; thermodynamics.

The liquid junction potentials in KCl, NaCl, and HCl concentration cells with transference have been evaluated by computer simulation, making use of Onsager flux coefficients tabulated by Miller, and of a convenient formalism for single-ion activity coefficients to make possible the representation of osmotic driving forces. Varying assumptions regarding single-ion activity coefficients lead to varying values of a computed steady-state junction potential, but these differences are canceled by corresponding differences in calculated electrode potentials, so that the computed overall cell potential remains unchanged—i.e., measurement of the potential of a concentration cell with transference can give no information about single-ion activity coefficients. This expected result plus the agreement of computed cell potentials with experimental ones speaks both for the essential validity of the method and for the mutual self-consistency of the numerical values inserted for Onsager coefficients and for mean ionic activity coefficients. In contrast to the steady-state cell potential, the time rise of the calculated potential is sensitive to the choice made for the single-ion activity coefficient parameter. There would thus seem to exist a possibility for determining single-ion activities in an experiment, if the time rise of the cell potential, after the formation of the junction, could be measured on a nanosecond time scale.

**12843.** Currie, L. A., **On the interpretation of errors in counting experiments**, *Anal. Lett.* **4**, No. 12, 873-882 (1971).

Key words: Activation analysis; Binomial and Poisson distributions; chi-squared; compound distributions; dispersion test; radioactivity.

Digital experiments, such as the measurement of radioactivity, are usually characterized by random errors which follow the Binomial or Poisson distribution. Three types of difficulty which commonly arise in the statistical treatment of such experiments include: (a) failure to recognize that the uncertainty in the physical quantity of interest may be governed by a compound probability distribution, particularly when dealing with short-lived radioactivity; (b) the improper use of the chi-squared statistic when making standard error estimates in weighted least-squares calculations; and (c) selecting the correct number of degrees of freedom and choosing between the  $\chi^2$  dispersion test and the goodness-of-fit test for grouped data. Examination of the nature of each of these difficulties has been followed by a recommended course of action.

**12844.** Carpenter, B. S., **Boron and uranium determination in simulated lunar glass by the nuclear track technique**, (Proc. American Nuclear Society 16th Annual Meeting, Los Angeles, Calif., June 28-July 2, 1970), *Trans. Amer. Nucl. Soc.* **13**, No. 1, 79 (1970).

Key words: Alpha particles; boron; fission; fragments; recoiling fission fragments; trace element glasses; uranium.

Recoiling fission fragments and alpha particles were used to determine sub-microgram quantities of uranium and boron in three (50, 1 and 0.02 ppm) Trace Element Glasses certified by the National Bureau of Standards. Procedures for preparing the sample, irradiating the sample in the NBS Reactor, counting and calculations of results are given.

**12845.** Kirstein, A. F., **Discussion of the paper "Behavior of fiber glass reinforced concrete beams"** by E. G. Nawy, G. E. Neu-

werth, and C. J. Phillips, *J. Struct. Div. Proc. Amer. Soc. Civil Eng.* **98**, No. ST5, 1206-1207 (May 1972).

Key words: Concrete (reinforced); deflection; disc; fiber glass; flexure; structural engineering.

**12846.** Plummer, E. W., Bell, A. E., **Field emission energy distributions of hydrogen and deuterium on the (100) and (110) planes of tungsten**, *J. Vac. Sci. Technol.* **9**, No. 2, 583-590 (Mar.-Apr. 1972).

Key words: Energy distribution; field emission; hydrogen; tungsten; tunneling.

Total energy distributions of field emitted electrons from the tungsten (110) and (100) planes as a function of coverage by hydrogen and deuterium have been recorded utilizing a spherical deflection energy analyzer. The elastic tunneling resonance spectrum gives a plot of the "local density of states" in the adsorbate. The inelastic tunneling spectrum reveals those discrete excitation energies available in the adsorbate—substrate complex. These spectroscopic data have been used to infer the chemical nature of the binding states which have been observed in the flash desorption spectrum of hydrogen from tungsten.

**12847.** Gadzuk, J. W., **Tunneling from Cambridge surface states**, *J. Vac. Sci. Technol.* **9**, No. 2, 591-596 (Mar.-Apr. 1972).

Key words: Field emission; metals; surface states; tunneling.

Solids with electron band structures given by a simple analytic function of wavenumber ( $E \sim k^2$  for free electron bands;  $E \sim k$  for tightbinding bands) possess localized electron states at their surfaces which are easily treated within the complex  $k$  vector formalism developed especially by Heine and collaborators. These surface states, which will be called Cambridge surface states, can occur not only in energy gaps caused by Bragg reflections at Brillouin zone faces but also in spin-orbit split gaps and hybridization gaps within the zone. In this work a theory of tunneling and field emission of electrons from such surface states is developed. The field emission energy distribution from  $d$ -band metal surface states is calculated using Harrison's  $d$ -band pseudopotential theory, and the results are favorably compared with experimental data. Since the existence conditions for Cambridge surface states depend crucially upon the boundary conditions at the surface, the act of measurement via a tunneling process can sufficiently alter the boundary conditions that "surface states" are either created or destroyed by "looking" at them. In particular the strong coupling ion neutralization tunneling experiments of Hagstrum are very susceptible to this effect.

**12848.** Marzetta, L. A., **An evaluation of the three-voltmeter method for ac power measurement**, (Proc. Conf. Digest on Precision Electromagnetic Measurement, Boulder, Colo., June 26, 1972), *IEEE Trans. Instr. Meas.*, pp. 41-42 (June 26, 1972).

Key words: Opamp; phase-sensitive detector; power-factor; quadrature; three-voltmeter method; wattmeter.

The accuracy and frequency response limitations in the present square-law responding laboratory wattmeters have promoted the search for alternate methods of ac power measurement using electronic instrumentation. The three-voltmeter method is based on an old principle of operation implemented by new analog circuitry. Results of the tests reported here show a precision of power calculation with 0.01% error at frequencies below 5 kHz. A unique test procedure is described for the comparison of the three-voltmeter device and a time-division multiplier wattmeter operating at zero power-factor.

**12849.** Lehman, D. R., **Quasielastic electron scattering from  $^3\text{He}$  and  $^3\text{H}$** , *Phys. Rev. C* **3**, No. 5, 1827-1840 (May 1971).

Key words: Electron scattering; final state rescattering; helium-3; separable potential; three-body problem; tritium.

Quasielastic electron scattering from  $^3\text{He}$  and  $^3\text{H}$  is investigated with a model in which the two-nucleon interaction is described by a separable potential. Cross sections are given in the impulse approximation for the ejected proton and scattered electron detected in coincidence, and for detection of only the scattered electron. Both two- and three-body breakup of  $^3\text{He}$  and  $^3\text{H}$  are considered, with final-state interactions between the spectator nucleons included in three-body breakup. Good agreement is obtained with all the electrodisintegration data, except the  $^3\text{He}$  coincidence data, for wave functions derived from separable potentials which reproduce the  $s$ -wave two-nucleon phase shifts at low and medium energies. Rescattering corrections between the spectator particles are found to be important in calculating three-body disintegration. The need for more refined and reliable coincidence data is reaffirmed.

**12850.** Menke, J. L., A fast pulse-dc integrator, *Nucl. Instrum. Methods* **64**, 61-68 (1968).

Key words: Fast integrator; high duty; integral linearity; stable converter; wide dynamic range.

This fast pulse-dc integrator accepts pulses from dc to less than 20 ns width, over an input dynamic range of 400:1 in amplitude (1 mV minimum) without range switching. The integral linearity (maximum absolute error as fraction of full scale) is 0.1 ppm at constant pulse height, 0.2% at constant pulse width. Any reading is accurate to within 2%. Temperature compensation and dc feedback ensure stability of operation. A fast voltage-to-current converter stable to 0.002% of full scale current provides the charge for capacitor storage.

**12851.** Shah, J. A., Danos, M., Study of the neutron-proton correlations in the shell model, *Phys. Rev.* **183**, No. 4, 899-907 (July 20, 1969).

Key words: Correlations; neutrons; pairing; quartetting; shell-model; structure; wave function.

A shell-model treatment is given for the spectra of the nuclei where there are two protons and two neutrons outside a doubly closed shell. The only restriction is that like-nucleons are required to occupy the same angular momentum state. In addition to this general wave function, more restricted wave functions also are investigated, viz., the pairing wave function (as least one pair of like nucleons is coupled to zero angular momentum) which contain no  $n$ - $p$  correlations; the quartetting wave function (two unlike nucleons are first coupled to the maximum angular momentum, then the two pairs are coupled to  $I$ , the nuclear angular momentum) which does contain  $n$ - $p$  correlations; and a superposition of pairing and quartetting wave functions. Results for  $^{44}\text{Ti}$ ,  $^{64}\text{Zn}$ , and  $^{204}\text{Hg}$  are given. The ground states are reproduced quite well by the pairing wave function; it seems, however, to fail for the excited states. The overlap between the general and the quartetting wave function is quite large. Finally, results are also given for the pairing force, which has only a  $T=1$  component.

**12852.** Casella, R. C., Time reversal symmetry and its breaking in physics, *Phys. Teacher* **8**, No. 3, 114-122 (Mar. 1970).

Key words: CP symmetry; CPT theorem; elementary particles;  $K^0$  mesons; symmetry; time reversal.

We remark on the relevance of symmetries in Nature, with emphasis on time reversal symmetry, its meaning, relation to other symmetries, and its experimental breakdown in elementary-particle physics.

**12853.** Lightbody, J. W., Jr., Penner, S., Electroexcitation of the  $\text{C}^{12}$  giant resonance, *Phys. Rev. Lett.* **24**, No. 6, 274-276 (Feb. 9, 1970).

Key words: Electroexcitation; energy dependent potential; Goldhaber-Teller model; longitudinal; matrix elements; momentum transfer; particle-hole model; quasi-elastic model; radiation tail; transverse.

Electroexcitation of  $\text{C}^{12}$  in and above the giant resonance has been measured at several angles and incident electron energies in order to obtain transverse and longitudinal reduced matrix elements. Results are presented for a  $q$  range of from 0.35 to 0.84  $\text{fm}^{-1}$  and for excitation of 22-37 MeV. Comparison is made with the recent calculation by deForest of quasielastic scattering, as well as with earlier particle-hole and liquid-drop-model calculations.

**12854.** Mohan, R., Danos, M., Biedenharn, L. C., Three-fluid hydrodynamical model and the proton distribution in  $^{208}\text{Pb}$ , *Phys. Rev. Lett.* **23**, No. 15, 868-870 (Oct. 1969).

Key words: Electron scattering; hydrodynamic model; isospin mixing; nuclear charge distribution; nuclear structure; short range correlations.

A three-fluid hydrodynamical model for nuclei is proposed and it is shown that the observed rise in proton density near the surface of  $^{208}\text{Pb}$  can be accounted for in this model.

**12855.** Wyckoff, J. M., Integrated cross sections for  $^{209}\text{Bi}(\gamma, xnyp)$  reactions, *Phys. Rev.* **159**, No. 4, 953-954 (July 20, 1967).

Key words: Bismuth; gamma rays; integrated cross section; isomer; lead; linac; lithium drifted germanium; photonuclear; spallation.

Integrated cross sections for the photoproduction of  $^{200-206}\text{Bi}$  and  $^{200-204}\text{Pb}$  from  $^{209}\text{Bi}$  have been measured. A single sample was activated during a 10-minute 137-MeV bremsstrahlung bombardment by the NBS Linac, and  $\gamma$  rays from the daughter products were measured with a Ge(Li) spectrometer over a two-month period to obtain relative yields. The yield data were used along with the established  $(\gamma, 2n)$  integrated cross section and a calculated thick-target bremsstrahlung spectrum to derive integrated cross sections as follows:  $^{206}\text{Bi}(168 \pm 25)$ ,  $^{205}\text{Bi}(88 \pm 22)$ ,  $^{204}\text{Bi}(55 \pm 16)$ ,  $^{203}\text{Bi}(66 \pm 23)$ ,  $^{202}\text{Bi}(31 \pm 12)$ ,  $^{201}\text{Bi}(10.7 \pm 5.9)$ ,  $^{200}\text{Bi}(5.7 \pm 3.4)$ ,  $^{204}\text{Pb}(8.0 \pm 2.4)$ ,  $^{203}\text{Pb}(3.8 \pm 1.3)$ ,  $^{202}\text{Pb}(3.4 \pm 1.3)$ ,  $^{201}\text{Pb}(15.3 \pm 8.4)$ , and  $^{200}\text{Pb}(1.62 \pm .97)$  MeV mb. Evidence is also presented for an 11.5-h isomeric state in  $^{200}\text{Pb}$ .

**12856.** Wyckoff, J. M., Photon energy emission from spallation products produced by 3-13 GeV electrons, *Health Phys.* **18**, 693-704 (June 1970).

Key words: Photon energy; production cross sections; spallation products; 3-13 GeV electron beam.

A calculation of the energy emitted as photons from the ensemble of spallation products produced by a 3-13.3 GeV electron beam has been made. The time range of 1 hr-50 months after irradiation is encompassed using measured production cross sections for Al, Fe, Ni and Cu, major structural materials used around high energy particle accelerators. Similar calculations have been made for Mo, In, Ta and Pb by estimating production cross sections for some of the nuclides for which measured production cross sections were not available. Additional production cross sections measured for 3, 5 and 10 GeV electrons and comparisons with published 3-30 GeV proton spallation data are used to show the general applicability of the calculated decay curves. Graphs of the instantaneous irradiation case are included as well as some illustrative results for photon energy emitted following extended irradiation periods.



**12857.** Praderie, F., Thomas, R. N., **On estimates of the nonradiative energy input to the solar chromosphere from the H<sup>-</sup> emission**, *Astrophys. J.* **172**, No. 2, 485-490 (Mar. 1, 1972).

Key words: H<sup>-</sup> radiative losses; non-LTE effects on mechanical heating; solar chromospheres.

The inclusion of non-LTE effects in the computation of mechanical heating in a gray atmosphere changes previous LTE estimates by a factor of  $4b_H$ .

**12858.** O'Toole, W. E., III, Keplinger, M. S., **An experimental program for automatic indexing at the National Bureau of Standards**, *Proc. American Society for Information Science, Philadelphia, Pa., Oct. 11-15, 1970*, **7**, 301-308 (American Society for Information Science, Washington, D.C., Oct. 1970).

Key words: Automatic indexing; COBOL; document records; programming; statistical analysis; teaching sample; word-term pairing.

A simple approach to automatic indexing is described along with its implementation in a program system.

The two main programs of the system, TESAT and IBSAT, are described from an operating point of view. The background is given for the development of the system, CAIC (Computer-Assisted Indexing and Categorizing). Also included are brief descriptions of experiences with the system and possible future applications and modifications.

**12859.** Holt, H. K., Sellin, I. A., **Time-dependent theory of Stark quenching of 2S states in hydrogen and helium**, *Phys. Rev. A* **6**, No. 1, 508-512 (July 1972).

Key words: Lifetimes; one- and two-electron 2S states; Stark quenching; time-dependent theory.

A nonperturbative time-dependent theory which gives Stark-quenching lifetimes in agreement with experiment for both one- and two-electron 2S states is presented. This theory differs from the conventional Bethe-Lamb theory of Stark quenching, but reduces to this older theory, for one electron atoms only, when a well-known sum rule is applied.

**12860.** Wyckoff, H. O., Rossi, H. H., **Dosimetric fundamentals and irradiation limits. I.1. Radiation quantities and units**, Chapter 1 in *Engineering Compendium on Radiation Shielding I*, 1-5 (Springer-Verlag, New York, N.Y., 1968).

Key words: Definitions; glossary; radiation quantities; radiation shielding; radiation units.

This is part of an introduction to a book on radiation shielding. It includes definitions of quantities and units to be used in the book.

**12861.** Wachtman, J. B., Jr., Capps, W., Mandel, J., **Biaxial flexure tests of ceramic substrates**, *J. Mater.* **7**, No. 2, 188-194 (1972).

Key words: Aluminum oxide; bending; brittleness; ceramics; electronics; flexural strength; fractures (materials); mechanical tests; modulus of rupture tests; substrates; surface properties.

A method for determining the strength of thin, circular disks of brittle materials utilizing an exact elastic solution for small deflections was developed and tested in an interlaboratory program. The method determines the strength in biaxial flexure by supporting the specimen on three equally spaced balls concentric with the load, which is applied to the center of the specimen by a flat piston. This allows slightly warped specimens to be tested and produces results unaffected by the edge condition of the

specimen. These features make the method suitable for assessing the effect of surface condition on strength. Results on eight types of polycrystalline alumina ceramics ranging in strength from 46,000 to 96,000 psi show that a coefficient of variation of about seven percent can be achieved by testing five specimens and that different laboratories generally obtain good agreement on strength values.

**12862.** Hanley, H. J. M., Klein, M., **Application of the m-6-8 potential to simple gases**, *J. Phys. Chem.* **76**, No. 12, 1743-1751 (1972).

Key words: Carbon dioxide; diffusion; dispersion coefficients; methane; m-6-8 potential; nitrogen; oxygen; rare gases; thermal conductivity; thermal diffusion; viscosity.

The m-6-8 model potential function is applied to the gases argon, krypton, xenon, nitrogen, methane, and carbon dioxide and to the properties viscosity coefficient, self-diffusion coefficient, thermal conductivity coefficient, virial coefficient, and the isotopic thermal diffusion factor. The potential is shown to have a considerable advantage over previous simple analytic models in that it can satisfy two criteria: (a) it can be used to correlate a given property for all the gases studied over a wide temperature range with a single set of parameters, and (b) it can be used to correlate both transport and equilibrium properties for the monatomic gases with a single set of parameters. Reasons for the failure of polyatomic gases to satisfy (b) are suggested. A brief discussion on the relation of the potential to theory is given.

**12863.** Spencer, L. V., **On the accuracy of transport calculations using moments methods**, *Trans. Amer. Nucl. Soc.* **14**, No. 1, 339 (June 1971).

Key words: Biorthogonal functions; gamma rays; moments methods; neutrons; shielding; truncation errors.

Expressions are given for bounds to the truncation error of finite  $U_n^k$  polynomial representations of  $\gamma$ -ray and neutron spatial flux distributions. An extension to representations of a class including sums of exponentials is also noted.

**12864.** Leiss, J. E., **Beam loading and transient behavior in traveling wave electron linear accelerators**, Chapter in *Linear Accelerators*, P. M. Lapostolle and A. L. Septier, eds., pp. 147-172 (North-Holland Publ. Co., Amsterdam, The Netherlands, 1970).

Key words: Accelerators; beam loading; dispersive effects; linear accelerator; transients.

In the linear accelerator the transfer of energy from the accelerator to the beam, known as beam loading, can be so efficient that the behavior of the accelerator can not be even qualitatively described without consideration of beam loading. The energy of loading, and changes in the radio frequency power density at some points in the accelerating waveguides of an order of magnitude are observed.

A review of methods to calculate beam loading in the traveling wave linear accelerator is presented. Both steady state and transient conditions are examined in various approximations.

**12865.** Swartzendruber, L. J., Evans, B. J., **Hyperfine fields at the antimony sites in the Heusler-type  $\text{Ni}_x\text{MnSb}$  alloys**, (Proc. 17th AIP Conf. on Magnetism and Magnetic Materials, Chicago, Ill., Nov. 15-18, 1971), Chapter in *Magnetism and Magnetic Materials*, C. D. Graham, Jr., and J. J. Rhyne, eds., No. 5, 539-543 (June 1972).

Key words: Alloys; hyperfine fields; Mössbauer effect; order-disorder;  $^{121}\text{Sb}$ .

The  $^{121}\text{Sb}$  Mössbauer effect has been utilized to study hyperfine fields in the ferromagnetic alloys  $\text{Ni}_x\text{MnSb}$  for  $1 \leq x \leq 2$ . For  $x=2$ , the crystal structure is of the  $\text{Cu}_2\text{MnAl}$  ( $\text{L2}_1$ ) type characteristic of Heusler alloys. As  $x$  is reduced, Ni vacancies appear until, for  $x=1$ , the ordered  $\text{C}_{16}$  structure is obtained. Our results indicate a  $^{121}\text{Sb}$  saturation magnetic hyperfine field of approximately +300 kG with a relatively small dependence on Ni concentration. It is possible to understand this result by using two assumptions: (i) the Ni atoms make only a small contribution to the conduction band and (ii) the Sb hyperfine field samples the average spin polarization of the material. The Mössbauer spectra form a sensitive probe to reveal disorder not easily observed by x-ray diffraction. A spin-echo measurement of  $^{121}\text{Sb}$  in  $\text{NiMnSb}$  gives good agreement with the  $^{121}\text{Sb}$  Mössbauer effect results.

**12866.** Swartzendruber, L. J., Bennett, L. H., Kinsman, K. R., *Crystallographic and magnetic transformations of Fe precipitates in Cu*, (Proc. 17th AIP Conf. on Magnetism and Magnetic Materials, Chicago, Ill., Nov. 15-18, 1971), Chapter in *Magnetism and Magnetic Materials*, C. D. Graham, Jr., and J. J. Rhyne, eds., No. 5, 408-412 (June 1972).

**Key words:** Alloys; copper; crystallography; iron, Mössbauer effect; precipitation.

The Mössbauer effect has been used to characterize the magnetic state, and hence the crystallographic form, of very small Fe-rich precipitates extracted from a Cu matrix. The precipitates form in the Cu matrix as antiferromagnetic (Néel temperature  $\sim 60$  K) metastable fcc crystals. When this two phase matrix is deformed or the precipitates selectively isolated from the matrix, a portion of the precipitates spontaneously transform (martensitically), at least partially, to bcc Fe. By a newly developed procedure we have extracted these fcc precipitates from the matrix, collected, and mounted them for observation by Mössbauer spectroscopy. The samples observed consist of small particles of Fe, containing  $\sim 0.5\%$  Cu, in the size range 0.1-0.2  $\mu\text{m}$ . Since the fcc and bcc crystal structures of Fe have widely different magnetic properties, the Mössbauer effect can be used to quantitatively characterize the crystallographic transformation. In the extracted precipitates conversion to bcc is essentially complete, in contrast to the only partial transformation induced by deformation. An upper limit ( $< 0.3\%$ ) can be placed on the amount of retained antiferromagnetic phase.

**12867.** Sharp, K. G., Coyle, T. D., *Perfluoro(alkylsilanes). II. Trifluoro(trifluoromethyl)silane and trifluoro(pentafluoroethyl)silane*, *Inorg. Chem.* 11, 1259-1264 (1972).

**Key words:** Alpha-elimination; carbenes; difluorocarbene; difluoroiodo(perfluoroalkyl)silanes; fluoroalkylsilanes; fluoro(trifluoromethyl)carbene; silicon difluoride; trifluoro(pentafluoroethyl)silane; trifluoro(trifluoromethyl)silane.

The perfluoro(alkylsilanes)  $\text{CF}_3\text{SiF}_3$  (I) and  $\text{C}_2\text{F}_5\text{SiF}_3$  (II) have been prepared and characterized. Synthesis was effected by fluorination of the corresponding difluoroiodo(perfluoroalkyl)silanes, obtained by the reaction of  $\text{SiF}_2$  with the appropriate perfluoroalkyl iodide. Both compounds are stable at room temperature. Products from thermolysis of I at *ca.* 80° or above and of II at 160° or above, as pure compounds or in the presence of added reagents, are consistent with a decomposition mechanism involving  $\alpha$ -fluorine transfer and the intermediacy of the carbenes  $:\text{CF}_2$  and  $\text{CF}_3\text{CF}$ , respectively. Basic and aqueous hydrolytic behaviors are described.

**12868.** McMaster, W. H., Del Grande, N. K., Mallett, J. H., Hubbell, J. H., *Compilation of x-ray cross sections, Sec. II, Rev. 1, University of California Radiation Laboratory Report*

50174, 353 pages, Lawrence Livermore Laboratory, Livermore, Calif. (May 1969).

**Key words:** Attenuation coefficient; coherent scattering; compilation; cross section; incoherent scattering; photoelectric absorption; photons; x-rays.

This report contains graphs and tables of x-ray cross sections in the range of 1 keV to 1 MeV. The total cross sections presented are the sum of computed scattering cross sections and a combination of the fit to derived experimental and theoretical photoelectric cross sections.

**12869.** Dikkers, R. D., Yokel, F. Y., *Strength of brick walls subject to axial compression and bending*, (Proc. 2d International Brick Masonry Conf., Stoke-on-Trent, England, Apr. 12-15, 1970), Chapter in *SIBMAC Proceedings*, H. W. H. West and K. H. Speed, eds., No. 19, 125-132 (The British Ceramic Research Association, Stoke-on-Trent, England, 1971).

**Key words:** Brick walls; combined loading; compressive strength; flexural strength; high bond mortar; masonry walls; moment magnifier effect; slenderness effects; structural stability.

Unreinforced brick wall panels, 4-in. thick, 4-ft wide, and 8-ft high, were tested by applying uniform transverse loads, uniform axial compressive loads, or a combination of both types of loading. Companion prisms were also tested to determine their strength in compression and flexure. Data from both the wall and prism tests were used to develop analytical procedures for predicting the strength of walls subjected to axial compression and bending.

A new analytical approach is proposed to evaluate both strength and slenderness effects in masonry walls. The application of this approach would lead to new design procedures, closely paralleling similar procedures recently introduced in the USA for other engineered materials, such as steel and reinforced concrete.

**12870.** Rowen, J. W., Murphey, W. M., Smith, C. N., *Assessment of material unaccounted for control criteria*, (Proc. Synp. Progress in Safeguards Techniques, International Atomic Energy Agency, Vienna, Austria, 1970), Chapter in *Safeguards Techniques II*, 291-310 (Dec. 1970).

**Key words:** Inventory fluctuations; measurement errors; normalization factors; process activity; unidentified process losses.

Some of the factors that affect the usefulness of Material Unaccounted For (MUF) control criteria include process activity, measurement errors, normalization factors, time frame, inventory fluctuations and unidentified process losses.

It is important to know whether and how such criteria vary with the character of the data source and with variations in facility situations. This paper theoretically analyzes MUF criteria corresponding to three types of data sources and two situations. The two situations differ in that measurement errors are known in one but unknown in the other. Quantitative criterion expressions are developed for the six possible conditions of evaluation resulting from the three types of data sources and the two measurement situations. The statistical expressions developed are compared with each other and some available data are presented. Tentative conclusions are drawn with respect to the comparative sensitivities of the criteria resulting from the six possibilities. These conclusions will be tested in the U.S. Atomic Energy Commission's integrated safeguards experiments. These experiments which will provide data for some of the situations will involve subprocess, batch and campaign balances in which information on measurement errors will be available.



**12871.** Kidnay, A. J., Miller, R. C., Hiza, M. J., **Solid-vapor and liquid-vapor phase equilibria for the helium-krypton system**, *Ind. Eng. Chem. Fundam.* **10**, No. 3, 459-465 (Aug. 1971).

Key words: Cryogenic; helium-krypton; liquid-vapor; phase equilibria; solid-vapor.

A vapor-recirculation equilibrium cell was used to investigate both the solid-vapor and liquid-vapor equilibria and the three-phase curve for the system helium-krypton. Gas-phase compositions were measured above solid krypton at 100.00, 105.00, 110.00, and 115.00 K and at pressures to 120 atm (12.16 MN/m<sup>2</sup>). Both gas and liquid compositions were determined at 117.09, 120.85, 129.60, 139.56, and 150.00 K for the same range of pressures. Analysis of the gas-phase data by both the virial and modified Redlich-Kwong equations indicates that a deviation parameter of about 0.3 is necessary for the geometric-mean mixing rule for energy parameters. Comparison of the Henry's law constants for the liquid phase with the statistical model of Miller and Prausnitz indicates a somewhat larger deviation parameter.

**12872.** Eisenhauer, C., **Some current problems in OCD fallout shielding calculations**, *Proc. Special Sessions on Gamma-Ray Production and Transport and on Civil Defense Shielding, Winter Meeting American Nuclear Society, Chicago, Ill., Nov. 1967*, A. E. Straker, ed., ANS-SD-7, (TID) 4500, pp. 143-156 (1969).

Key words: Civil Defense; engineering method; fallout; gamma rays; shelter; shielding.

A discussion is given of the general situations in which present OCD calculations seem to be adequate. This consists mainly of the case in which an infinite plane source of radiation surrounds a simple building with no interior walls or floors. Three cases in which present calculations appear to be inadequate will be discussed in detail. The first case in which calculations appear to be inadequate involves a finite source strip whose width is a few story heights (~ 50 feet). The two main problems are that the theory assumes that radiation emerging from the inner surface of the exterior walls is symmetric with respect to the horizontal plane, and that the barrier factor for radiation penetrating up through the floor is equivalent to the barrier factor for a plane isotropic source. Possible modifications of these two assumptions are discussed. The second case is the "in-and-down" problem, in which radiation from sources on the ground penetrates *in* through a wall and *down* through the basement ceiling. The two main problems here are that the variation of reduction factor with depth is incorrect and that experimental results on model and full-scale structures given barrier factors which are in apparent disagreement. A possible explanation of this disagreement is discussed, along with some recent experimental data. The third case in which calculations seem to be inadequate is that of a core shelter. This situation occurs when interior partitions are significantly greater than a mean free path in thickness. The particular case of a home fallout shelter in a basement is discussed. The paper concludes with a summary of plans for experiments and calculations in the near future.

**12873.** Johnson, W. T. K., Dick, C. E., **Half-life measurement of several short-lived nuclear isomers**, *Nucl. Instrum. Methods* **99**, No. 2, 221-226 (1972).

Key words: Bromine; cadmium; erbium; gold; half lives; iridium; measurement; nuclear isomers; solenium; tungsten.

Bremsstrahlung produced by 3.5 MeV electrons incident on a platinum target was used to populate nuclear isomers in several nuclei through excitation of higher lying states. A shuttle was constructed to transport targets of natural isotopic abundance from an irradiation position to a measuring position. Other than

a low background the activity measured was due entirely to the isomeric decay. The measured half-lives in seconds are <sup>77m</sup>Se:  $17.58 \pm 0.12$ , <sup>79m</sup>Br:  $4.97 \pm 0.10$ , <sup>167m</sup>Er:  $2.28 \pm 0.03$ , <sup>179m</sup>Hf:  $18.77 \pm 0.07$ , <sup>183m</sup>W:  $5.56 \pm 0.25$ , <sup>191m</sup>Ir:  $4.88 \pm 0.03$ , and <sup>197m</sup>Au:  $7.86 \pm 0.04$ . The data are presented and the methods of analysis are discussed. The results are compared to recent literature values.

**12874.** Kondo, A., Brenner, F. C., **Research for a uniform quality grading system for tires. VI. Comparison of the effect of front and rear wheel drive vehicles on projected tread wear of a tire**, *Rubber Chem. Technol.* **44**, No. 4, 960-961 (Sept. 1971).

Key words: Automobile tires; environment; grading; pavement; rating; test method; tread wear.

The total number of miles that could be expected for a tire was projected and compared from a test involving a front axle drive and a rear axle drive vehicle. On the front axle drive vehicle the tires wore at twice the rate on the front wheels as on the rear; on the other vehicle they wore at about the same rate on both axles.

The projected mileages for the tires on the two vehicles were 22,400 and 22,500 miles which is not significantly different.

**12875.** Linzer, M. A., **A frequency swept injection locked nuclear induction spectrometer with signal averaging**, *Rev. Sci. Instrum.* **43**, No. 5, 723-726 (May 1972).

Key words: Frequency-sweep; injection-locking; nmr; nqr; nuclear induction; signal averaging.

A frequency sweep injection technique, suitable for signal averaging and fast passage studies, has been developed for use with a nuclear induction spectrometer.

**12876.** Treu, S., **A conceptual framework for the searcher-system interface**, *Proc. Workshop on Interactive Bibliographic Search: The User/Computer Interface, Palo Alto, Calif., Jan. 14-15, 1971*, D. E. Walker, ed., pp. 53-66 (AFIPS Press, Montvale, N.J., 1971).

Key words: Bibliographic search; conceptual framework; interactive search system; man-computer interaction; man-machine system.

A conceptual framework for the searcher-system interface is portrayed as dependent on whether (and how) the real or virtual capabilities of the search system can satisfy the natural characteristics of human interactive information-seeking behavior. A pragmatic retain-rectify-reform approach is defined and carried out towards arriving at a set of twelve such characteristics. Because empirical confirmation (or rebuttal) is desirable but lacking, a "transparent stimulation" experiment is suggested and broadly described.

**12877.** Petrescu-Prahova, I., Winogradoff, N. N., **Photoluminescence in compensated n-type, Si-doped gallium arsenide**, *J. Phys. Chem. Solids* **32**, 1873-1879 (1971).

Key words: Amphoteric compensation; band tailing; coulomb potential screening; gallium arsenide; photoluminescence; silicon doping.

Band tailing observed in highly doped GaAs and other semiconductors has been attributed to screened coulomb potentials. The amphoteric nature of melt-grown, Si-doped samples, limiting the free electron concentration to below  $n = 5 \times 10^{18}$  cm<sup>-3</sup>, permitted the unequivocal study of the band tail parameters as a function of impurity concentration at virtually constant free carrier screening over a silicon concentration range from  $2.6 \times 10^{18}$  to  $1.2 \times 10^{20}$  cm<sup>-3</sup>. The photoluminescent spectra of such samples consisted of two broad bands, one of which, centered at 1.2 eV, decreased with increasing temperature and vanished at

the higher temperatures where accurate analysis of the shape of the other band, centered at any energy close to the band gap, could be made. The intensity of the low energy side of the latter band was found to be exponential proportional to  $\exp(h\nu/E_0)$ , and the dependence of  $E_0$  on the concentration of the silicon dopant was determined. Since a change of the excitation intensity over two orders of magnitude did not change the position or shape of the band-to-band "line," it was concluded that the nature of the spectra reflects exponential density-of-states tails at the conduction band edge.

12878. Skopik, D. M., Dodge, W. R., <sup>4</sup>He(*e,d*)*e'*<sup>2</sup>H angular-distribution and cross-section measurements between 36 and 50 MeV, *Phys. Rev. C* **6**, No. 1, 43-53 (July 1972).

Key words: E-2 angular distributions; electric-quadrupole transition; identical particles; virtual photons; <sup>4</sup>He photodisintegration.

Measurements of the angular distributions in the "virtual photon" energy interval of  $40 \pm 1$  MeV and the total cross section in the energy interval of 35.7 – 49.4 MeV of the <sup>4</sup>He(*e,d*)*e'*<sup>2</sup>H reaction are presented. The data are compared with early calculations and with more recent cluster-model and dispersive calculations.

12879. Robertson, A. F., Discussion of paper "Fire and the curtain wall" by H. L. Malhotra, United Kingdom, (Proc. Symp. of CIB Conf. on Curtain Walls, Paris, France, Mar. 3-6, 1970), *Symp. Papers in Light Facades*, pp. 74-75 (June 1971).

Key words: Curtain walls; exterior walls; fire spread.

The paper, "Fire and the Curtain Wall" by H. L. Malhotra to be presented in a symposium sponsored by Conseil International du Batiment pour Reserche et Documentation on the curtain wall has been discussed in the light of information currently available in the USA. It is suggested that the experiments quoted by Malhotra may have failed to properly simulate fire behavior in buildings of conventional shape. A word of caution is offered against the proposal that current code requirements with respect to height of spandrel walls or horizontal floor projections are unduly restrictive.

12880. Caswell, R. S., Review of measurements of absolute neutron emission rates and spectra from neutron sources, (Proc. Amer. Nucl. Soc. National Topical Meeting on Neutron Sources and Applications, Augusta, Ga., Apr. 19-21, 1971), Chapter in *Neutron Sources and Applications*, CONF-710402, I, 1-53 – 1-62 (1971).

Key words: Manganous sulfate bath; neutron emission rate; neutron sources; neutron spectra; neutron spectrum measurement methods; <sup>252</sup>Cf.

The measurement of the absolute neutron emission rate of neutron sources has been reviewed with emphasis on the manganous sulfate bath method, and is found to be in good quantitative shape. In precision applications, such as  $\nu$  (neutrons/fission) and certain cross section measurements, higher accuracy would, nevertheless, be desirable. Significant improvement in the accuracy of ( $\beta$ , n) source calibrations could be obtained by resolution of the discrepancy on the magnitude of the fast neutron loss to nuclear reactions in the manganous sulfate bath.

Recent developments in the techniques of measuring spectra of neutron sources has led to the beginning of reliable measurements in the energy region below 1 MeV. The source spectrum measurement field is, nevertheless, in semi-quantitative state. Further intercomparisons of measurement methods are needed, and also, the resolution of a discrepancy on the neutron energy spectrum for the <sup>252</sup>Cf spontaneous fission neutron source.

12881. Jacox, M. E., Milligan, D. E., Vibrational and electronic spectra of the O<sub>3</sub><sup>-</sup> anion isolated in an argon matrix, *J. Mol. Spectrosc.* **43**, No. 1, 148-167 (July 1972).

Key words: Charge transfer; electron attachment; infrared spectrum; matrix isolation; molecular orbitals; O<sub>2</sub> + O<sup>-</sup> reaction; O<sub>3</sub><sup>-</sup> anion; ultraviolet spectrum.

The O<sub>3</sub><sup>-</sup> anion has been stabilized in an argon matrix at 14 K in concentration sufficient for the detection of the antisymmetric stretching fundamental,  $\nu_3$ , and of a band system between 5100 and 3700 Å. Both the reaction of O<sup>-</sup> (produced by the interaction of photoelectrons with N<sub>2</sub>O) with O<sub>2</sub> and the charge-transfer interaction between O<sub>3</sub> and K atoms have served as sources of O<sub>3</sub><sup>-</sup> in these studies. Although the  $\nu_3$  absorption is slightly dependent upon the alkali metal used as the photoelectron source, the experiments suggest that the  $\nu_3$  absorption of P<sub>3</sub><sup>-</sup> isolated in an argon lattice should lie very close to 800 cm<sup>-1</sup>. Detailed isotopic studies support the proposed vibrational assignment and demonstrate that the valence angle of ground-state O<sub>3</sub><sup>-</sup> is  $110 \pm 5^\circ$  and that the oxygen-oxygen bonds are considerably weaker than those of O<sub>3</sub>. The nature of the observed electronic transition of O<sub>3</sub><sup>-</sup> is discussed, and evidence is considered for the presence of a low-lying dissociative state.

12882. Celotta, R. J., Bennett, R. A., Hall, J. L., Siegel, M. W., Levine, J., Molecular photodetachment spectrometry. II. The electron affinity of O<sub>2</sub> and the structure of O<sub>2</sub><sup>-</sup>, *Phys. Rev. A* **6**, No. 2, 631-642 (Aug. 1972).

Key words: Electron affinity; molecular constant; molecular oxygen; negative ions, photodetachment.

A beam of O<sub>2</sub><sup>-</sup> ions, extracted from a glow discharge in N<sub>2</sub>O, is crossed with the linearly polarized intracavity photon beam of an argon-ion laser (4880 Å). Electrons photodetached at right angles to the crossed beams are energy filtered by a hemispherical analyzer. The electron energy spectra are characteristic of photodetachment from the  $v' = 0$  state of O<sub>2</sub><sup>-</sup> to the  $X^2\Sigma_g^-$  and  $a^1\Delta_g$  state of O<sub>2</sub>. Vibrational state analysis is facilitated by the use of isotopes. The electron affinity obtained is  $0.440 \pm 0.008$  eV. Additionally, we have measured the relative transition probabilities as a function of final vibrational state and the angular distributions of the outgoing electrons. The relative intensities, corrected by the angular distributions, determine through Franck-Condon-factor analysis the internuclear distance for the negative ion. We find  $r_e^- = 1.341 \pm 0.010$  Å and therefore  $B_e^- = 1.17 \pm 0.02$  cm<sup>-1</sup>.

12883. Siegel, M. W., Celotta, R. J., Hall, J. L., Levine, J., Bennett, R. A., Molecular photodetachment spectrometry. I. The electron affinity of nitric oxide and the molecular constants of NO<sup>-</sup>, *Phys. Rev. A* **6**, No. 2, 607-631 (Aug. 1972).

Key words: Electron affinity; molecular constants; negative ions; nitric oxide; photodetachment.

We apply laser photodetachment and photoelectron spectrometry for the first time to the study of molecular negative ions. We describe in detail the study of the nitric oxide ion NO<sup>-</sup>; a following paper reports results for O<sub>2</sub><sup>-</sup>. We use the NO<sup>-</sup> results to develop and illustrate in detail the principles and applications of the technique. A mass-selected NO<sup>-</sup> beam (680 eV) is crossed with a linearly polarized monochromatic (4880-Å) argon-ion laser beam, and electrons photodetached into a  $4\pi/2000$ -sr solid angle perpendicular to the crossed beams are energy analyzed using a hemispherical electrostatic monochromator. The data yield a set of vertical detachment energies between vibrational states of NO<sup>-</sup> and NO, and relative intensities for these transitions. Angular distributions about the polarization direction are studied by rotating the laser polarization while maintaining the mutually perpendicular ion-beam-laser-beam-electron-collection



geometry. For each transition we measure the anisotropy parameter  $\beta$ , corresponding to the form  $[1 + \beta P_2(\cos \theta)]$  for the angular distribution. Several arguments, including data on NO<sup>18</sup>-photodetachment, are used to identify the initial and final vibrational states. Molecular rotational effects, and effects associated with the spin-orbit splitting of the final NO( $X^2\Pi$ ) state are identified and included in the analysis. A Franck-Condon-factor analysis of the observed relative cross sections, parametrized by trial values of the NO<sup>-</sup> molecular constants, is used to determine that for NO<sup>-</sup>  $\omega_e'' = 1470 \pm 200$  cm<sup>-1</sup>,  $r_e'' = 1.258 \pm 0.010$  Å, and  $B_e'' = 1.427 \pm 0.02$  cm<sup>-1</sup>. Using these constants, the measured vertical detachment energy is reduced by rotational and spin-orbit effects to the electron affinity  $E_A(\text{NO}) = 24_{-5}^{+10}$  meV.

**12884.** Utton, D. B., Tsang, T., **Coupled nuclear spin relaxation and internal rotations in magnesium fluosilicate hexahydrate**, *J. Chem. Phys.* **56**, No. 1, 116-119 (Jan. 1, 1972).

**Key words:** Internal motion; magnesium fluosilicate hexahydrate; nuclear magnetic resonance; relaxation.

Both proton and fluorine nuclear spin-lattice relaxations have been studied by the 180-90° pulse method in MgSiF<sub>6</sub>·6H<sub>2</sub>O at 25 and 13 MHz over the temperature range 170-350 K. Nonexponential behaviors have been observed. Both <sup>1</sup>H and <sup>19</sup>F relaxations may be characterized by the same pair of relaxation times, the shorter component due to the intermolecular H—F dipolar interaction. The results indicate that the SiF<sub>6</sub><sup>2-</sup> ions are reorienting with an activation energy,  $V = 31 \pm 4$  kJ/mole =  $7.5 \pm 1.0$  kcal/mole, and a frequency factor  $\tau_0 = 10^{-14 \pm 1}$  sec. These values are consistent with other hydrogen-bonded fluorine compounds.

**12885.** Hutchinson, J. M. R., Garfinkel, S. B., **Standardization of cadmium-109 sources for  $\gamma$ -ray emission rate**, *Int. J. Appl. Radiat. Isotop.* **22**, 405-414 (1971).

**Key words:** Cadmium-109; cobalt-57; gamma-ray emission rate; iron-57; photoelectron escape; silver-109M; standardization; well crystal counting.

The standardization of <sup>109</sup>Cd sources for 88-keV  $\gamma$ -ray emission rate has been performed using a NaI(Tl) well crystal which gives a nearly  $4\pi$  geometry. Since the low-energy portion of the 88-keV  $\gamma$ -ray spectrum is obscured by 22-keV X-ray pulses, the total counting rate cannot be found by merely summing the counting rates for all the channels in the distribution. A method, in which the spectrum is broken down into eight components, is used to determine the number of degraded 88-keV  $\gamma$ -ray pulses. The calibration is performed by summing the counting rates of the various components below an arbitrarily chosen energy of 39 keV, and adding them to the total counting rate above 39 keV. The process in which photoelectrons escape into the aluminum liner of the well is found to be responsible for most of the degraded 88-keV  $\gamma$ -ray pulses which fall below 39 keV. The estimated systematic error in the measurement is  $\pm 0.9$  percent.

Using <sup>57</sup>Co sources which have been accurately calibrated by coincidence counting, the 2-in.  $\times$  2-in. NaI(Tl) well crystal is shown to have a  $\gamma$ -ray detection efficiency of 100 percent with an uncertainty of  $\pm 0.2$  percent (after corrections have been made for well-wall  $\gamma$ -ray absorption and escape out of the well). The total abundance for 122- and 136-keV <sup>57</sup>Fe photons emitted per decay from <sup>57</sup>Co has been measured to be  $0.963 \pm 0.003$ .

**12886.** Hutchinson, J. M. R., Lantz, J. L., Mann, W. B., Mullen, P. A., Rodríguez-Pasqués, R. H., **An anti-coincidence shielded NaI(Tl) system at NBS**, *IEEE Trans. Nucl. Sci.* **NS-19**, No. 1, 117-118 (Feb. 1972).

**Key words:** Anti-coincidence; anti-Compton; gamma rays; low level radioactivity; multidimensional; radioactivity.

An anti-Compton, anti-coincidence shielded NaI(Tl) spectrometer is described.

**12887.** Rodríguez-Pasqués, R. H., **Microactivity radiochemistry**, *Proc. 2d Inter-American Conference on Radiochemistry, Mexico City, Mexico, Apr. 22-25, 1968*, pp. 278-289 (Published by Secretaría General de la Organización de Estados Americanos, Washington, D.C., 1971).

**Key words:** Detection limits; high sensitivity counting; low-level; low-level separations; microactivity; radiochemistry; radionuclide identification; specific activity threshold.

Microactivity is taken as synonymous with low-level radioactivity, and is defined as 1 dpm/g, or less. The refinements of technique developed to deal with these low levels have widened the field of radiochemical and nuclear chemistry research with new subjects. Two general requirements are discussed, namely high sensitivity detection, and refined chemical techniques.

The difficult problem of radionuclide identification at microactivity level is also examined.

**12888.** Hirshfeld, A. T., Hoppes, D. D., Mann, W. B., Schima, F. J., **Nuclear orientation of <sup>82</sup>Br in iron**, (Proc. Int. Conf. on Hyperfine Interactions in Excited Nuclei, Rehovot, Israel, Sept. 6-11, 1970), Chapter in *Hyperfine Interactions in Excited Nuclei* **1**, 335-338 (Gordon and Breach Sci. Publ., New York, London, Paris, 1971).

**Key words:** Beta rays; gamma rays; hyperfine interactions; isotope separator; magnetic moment; nuclear orientation; <sup>82</sup>Br.

<sup>82</sup>Br was implanted in .025 mm thick iron foil, using the NBS high-resolution isotope separator. The bromine was oriented by cooling by adiabatic demagnetization and the anisotropy of the emitted beta and gamma radiation observed. For the upper 40% of the 5<sup>-</sup>  $\rightarrow$  4<sup>-</sup> beta spectrum an asymmetry of  $\pm .046 \pm .004$  was observed at a foil temperature of 35 mK. This, taken together with the observed anisotropies for seven gamma peaks, indicates an effective field of  $400_{-100}^{+400}$  kG acting on a fraction of the bromine atoms. The sign of the <sup>82</sup>Br magnetic dipole moment is positive, assuming a positive value for the effective field.

**12889.** Soulen, R. J., Jr., Colwell, J. H., **The equivalence of the superconducting transition temperature of pure indium as determined by electrical resistance, magnetic susceptibility, and heat-capacity measurements**, *J. Low Temp. Phys.* **5**, No. 3, 325-333 (1971).

**Key words:** Carbon resistance thermometry; electrical resistance; heat capacity; indium; magnetic susceptibility; superconductivity; thermometric fixed point; transition temperature.

The superconducting transition temperature of a well-annealed polycrystalline sample of pure indium was determined by three different techniques. The heat-capacity and susceptibility transitions are approximately 1 mK wide and span the same temperature interval. The resistance transition is less than 0.2 mK wide and occurs at the center of the other transitions. By choosing the midpoint of each transition the three measurements are identical to within 0.1 mK.

**12890.** Cook, C. C., Allred, C. M., **An excitation system for piston attenuators**, *IEEE Trans. Instr. Meas.* **IM-20**, No. 1, 10-16 (Feb. 1971).

**Key words:** High-power impedance matching; mode filters; negative current feedback; waveguide-below-cutoff attenuator.

The problems of mode purity and the interaction effect generally necessitate a large insertion loss in precision waveguide-below-cutoff (piston) attenuators to obtain a linear output. An attenuator excitation system, used on a precision attenuation measuring system, that reduces these problems is described. Experimental work as well as theoretical considerations is discussed and designs are presented that have produced output voltages of the piston attenuator greater than 1 V while still maintaining a linearity of 0.001 dB as a function of piston position. This has been accomplished by (1) operating with large input power (100-200 W), (2) development of new exciting units with improved geometry for better field excitation and utilizing water-cooled elements for high-power operation, (3) special impedance matching networks having exceptional stability with high power input, (4) use of current feedback to achieve effectively constant current excitation, and (5) a mode filter that attenuates the undesired  $TE_{01}$  mode 98 dB while attenuating the desired  $TE_{11}$  mode only 0.2 dB.

**12891.** Gimmestad, G. G., Pardoe, G. W. F., Gebbie, H. A., **The study of dimeric molecules in ammonia vapour of submillimeter wave spectroscopy**, *J. Quant. Spectrosc. Radiat. Transfer* **12**, 559-567 (1972).

**Key words:** Ammonia; dimers; infrared.

Absorption by true dimers can be distinguished from that attributable to transient pairs by being spectrally narrow and by having a temperature dependence characterized by a well defined binding energy. Using these criteria, the presence of dimers in ammonia gas under conditions near those of saturated vapor is deduced from the observation of narrow spectral features near  $10\text{ cm}^{-1}$ , and a heat of dimerization of  $3.6 \pm 0.8$  kilocalories per mole. This value, of the order of what would be expected from breaking single hydrogen bonds, is a little lower than the values found by other methods. The presence of dimers should be considered in interpreting line shape observations at high pressures.

**12892.** Zimmerman, J. E., **Josephson effect devices and low-frequency field sensing**, *Cryogenics* **12**, No. 1, 19-31 (Feb. 1972).

**Key words:** Cryogenics; Josephson effect; magnetometry; superconductivity.

Three major areas of application of the Josephson effect are recognized; absolute standards, millimetre and sub-millimetre wave sensing, and dc and low-frequency current, voltage, and magnetic field sensing. In the latter area, single junction rf-biased low-inductance loop devices in a number of different forms (junction types and loop geometries) have been developed with sensitivities of the order of  $10^{-15}\text{ T}(10^{-11}\text{ G})$  or  $10^{-19}\text{ V}$ . These sensors are being used in applications as diverse as magnetocardiography and absolute noise thermometry in the millikelvin range. As amplifiers, they are characterized by demonstrated equivalent noise temperatures of less than a few millikelvin, and probably a few microkelvin (theoretical). Highly reliable thin-film loop devices in a number of different forms have been developed in several laboratories, but the more easily-made point-contact devices are probably the most widely used. Many of the characteristics of the devices can be easily interpreted with the aid of a pendulum analogue.

**12893.** Ruff, A. W., Jr., **Interpretation of x-ray diffraction data with regard to stacking faults in silver-tin alloys**, *J. Appl. Phys. Comm.* **43**, No. 6, 2909-2911 (June 1972).

**Key words:** Alloys; dislocation; stacking-fault energy; stacking-fault probability; x ray.

Several alternative interpretations of data from fcc silver-tin alloys are discussed in examining the relation between stacking-

fault probability and stacking-fault energy. One important aspect concerns the true variation of dislocation density with alloy composition.

**12894.** Siegwirth, J. D., Radebaugh, R., **The design of optimum heat exchangers for dilution refrigerators**, *Rev. Sci. Instrum.* **43**, No. 2, 197-204 (Feb. 1972).

**Key words:** Cryogenics; dilution refrigerator; heat exchangers; helium-3; helium-4.

The behavior of discrete heat exchangers as a function of temperature, heat transfer area, and  $^3\text{He}$  flow rate is shown for a general case by means of some machine calculated curves. From these curves, the appropriate heat exchanger size can be determined for the various steps of a discrete heat exchanger. Also, curves for the mixing chamber temperature  $T_m$  as a function of total surface area divided by flow rate for various amounts of external heat to the mixer are shown for the continuous exchanger. From these curves the optimum  $^3\text{He}$  flow rate for a given heat input and exchanger size can be determined. Viscous heating has been included in the calculation of one typical coaxial tube exchanger. It is found that heating in the dilute stream has negligible effect on  $T_m$ , whereas the viscous heating in the concentrated side, though several times smaller than that in the dilute side, has considerably more effect on  $T_m$ . Based on this behavior, an improved method of "heat sinking" heat leak paths to the mixer is suggested.

**12895.** Mizushima, M., Evenson, K. M., Wells, J. S., **Laser magnetic resonance of the NO molecule using 78-, 79-, and 119- $\mu\text{m}$   $\text{H}_2\text{O}$  laser lines**, *Phys. Rev. A* **5**, No. 5, 2276-2287 (May 1972).

**Key words:**  $g$  Factor; laser magnetic resonance; NO; spin-orbit coupling constant; water vapor laser.

The magnetic resonance of the NO molecule is observed using the 78-, 79-, and 119- $\mu\text{m}$  lines of the  $\text{H}_2\text{O}$  laser as the radiation source. The resonances in three cases are due to the  $(^2\Pi_{1/2}J=12.5) \rightarrow (^2\Pi_{3/2}J=12.5)$ ,  $(^2\Pi_{1/2}J=11.5) \rightarrow (^2\Pi_{3/2}J=11.5)$ , and  $(^2\Pi_{1/2}J=12.5) \rightarrow (^2\Pi_{3/2}J=11.5)$  transitions, respectively. Most of them are magnetic dipole transitions, but a few electric dipole transitions are also observed. It is found that the calculated  $g$  factors  $g_{c2}(11.5)=g_{d2}(11.5)=-0.0064$ ,  $g_{c1}(11.5)=g_{d1}(11.5)=0.0272$ ,  $g_{c2}(12.5)=g_{d2}(12.5)=-0.0092$ ,  $g_{c1}(12.5)=g_{d1}(12.5)=0.0270$ , and the calculated  $\Lambda$ -doublet separations  $f_{c2}(11.5)-f_{d2}(12.5)=243\text{ MHz}$ ,  $f_{c1}(11.5)-f_{d1}(11.5)=4323\text{ MHz}$ , are consistent with our experimental results. The hyperfine structure and the second-order effects are also in agreement with theoretical values. The average separation between the  $^2\Pi_{3/2}$  and  $^2\Pi_{1/2}$  states for a given  $J$ , which we call  $X_J$ , is found to be  $126.4469 \pm 0.0005$  and  $127.5786 \pm 0.0005\text{ cm}^{-1}$  for  $J=11.5$  and  $12.5$ , respectively. The conventional spin-orbit coupling constant is found to be  $123.1580 \pm 0.0010\text{ cm}^{-1}$  when  $J=12.5$  or  $11.5$ . [The conventional spin-orbit coupling constant  $A_c$ , commonly referred to as  $A$ , is given by  $A - \delta(J+1/2)^2 + 1/4\gamma$  in our notation.] The coupling constant  $\mu_s$  for the  $\vec{S} \cdot \vec{N}$  term is found to be  $-0.006 \pm 0.002\text{ cm}^{-1}$ .

**12896.** Prydz, R., Goodwin, R. D., **Experimental melting and vapor pressures of methane**, *J. Chem. Thermodyn.* **4**, No. 1, 127-133 (Jan. 1972).

**Key words:** Boiling point; critical-point pressure; melting pressure; methane; triple-point constants; vapor pressure.

Thirteen melting pressures to 210 atm are represented by the Simon equation with a root mean square deviation of 0.05 atm (0.08 percent). This representation is highly sensitive to the triple point temperature, yielding 90.680 K (IPTS-1968). These pressures agree within 0.5 percent with the less precise data of one other investigator at temperatures above 93 K. One hundred



and five vapor pressures from the triple point to the critical point are represented by a new, non-analytic equation with a root mean square relative deviation of 0.01 percent. The derived triple point pressure is 0.1159 atm. At the assigned critical point temperature of 190.53 K the pressure is 45.356 atm. Deviations of some of the data from other sources exceed one percent at  $T < 140$  K.

**12897.** Ledbetter, H. M., **An approximation of  $\theta_{\text{elastic}}$  for cubic metals**, *J. Phys. F* 2, No. 2, 262-269 (Mar. 1972).

Key words: Crystal properties; Debye temperature; elastic constants; velocity/elastic waves.

The Debye characteristic temperature  $\theta$  has been calculated from the elastic coefficients for 24 cubic elements by an approximate method proposed previously by other workers. The approximation requires that the elastic secular equation be solved only for the three principal cubic directions. New weighting coefficients for these directions were determined by a least squares best-fit procedure, based on computationally "exact" values of  $\theta$ . Comparisons with the results of previous three term approximations indicate which set of weighting coefficients gives the best approximation to  $\theta$ .

**12898.** McDonald, D. G., Risley, A. S., Cupp, J. D., Evenson, K. M., Ashley, J. R., **Four-hundredth-order harmonic mixing of microwave and infrared laser radiation using a Josephson junction and a maser**, *Appl. Phys. Lett.* 20, No. 8, 296-299 (Apr. 15, 1972).

Key words: Cryotemperatures; harmonic mixing; infrared detectors; Josephson junctions; laser frequency measurements; lasers; superconductivity.

For mixing in a Josephson junction at infrared frequencies, we have shown that the available power from the junction increases as the intermediate frequency is increased. Following this result an infrared receiver has been developed incorporating a 9-GHz maser preamplifier at the i.f. Using this system, the beat between the 401st harmonic of a high-quality microwave source and a 3.8-THz infrared laser has been observed. Also, for low-order mixing at 3.8 THz, a comparison of beat signals from a Josephson junction and a room-temperature mixer has been made.

**12899.** Ledbetter, H. M., Wayman, C. M., **The crystallography of the  $\beta$ -to- $\beta''$  AuCd martensitic transformation**, *Acta Met.* 20, No. 1, 19-30 (Jan. 1972).

Key words: Crystallography; gold-cadmium alloys; martensite; phase transformations.

The crystallography of the martensitic transformation in near-equiatomic AuCd alloys is re-examined, experimentally and theoretically, from the viewpoint that the low-temperature  $\beta''$  phase has either trigonal or hexagonal symmetry. The elements of the Bain strain accompanying the transformation are found to be smaller than those reported for any other metallic system. As a result, only the habit plane and the twin ratio are useful quantities for characterizing the transformation. Predictions of the present study are in accord with existing measurements of these quantities. The reported lattice correspondence is believed to be unique for the martensitic transformation of a beta phase alloy.

**12900.** Manning, J. R., **Impurity-correlation factors for diffusion in diamond-structure crystals**, *Phys. Rev. B* 6, No. 4, 1344-1355 (Aug. 15, 1972).

Key words: Correlation factor; diamond structure; diffusion; impurity; jump frequency; vacancy.

The correlation equations for impurity diffusion in the diamond structure have much in common with the equations for

self-diffusion in pure face-centered-cubic and diamond structures. Comparison of these equations allows the four-frequency expression for the impurity-correlation factor in the diamond structure to be calculated to the same precision as the correlation factor for self-diffusion in a pure face-centered-cubic structure. This precision is an order of magnitude better than that for any previous calculation of this impurity-correlation factor. The calculation also illustrates an effect that choice of diffusion direction can have on the form of the correlation-factor equations. In these calculations, a generalized method is developed of calculating impurity-correlation factors in terms of effective-vacancy-return probabilities  $U_q$ , including contributions from vacancies which move far away from the impurity before effectively returning to their original site. Connections between various calculational techniques are discussed. The accurate values obtained here are compared with previous calculations done by a variety of other methods. This allows an evaluation of the problems arising in various standard calculational techniques.

**12901.** Foote, W. J., Hunter, R. D., **Improved gearing for rotary-vane attenuators**, *Rev. Sci. Instrum.* 43, No. 7, 1042-1043 (July 1972).

Key words: Attenuator; microwave; rotary vane; Spiroid (Reg. T.M.).

A WR15 rotary-vane attenuator is modified and driven by a 180:1 precision gear set. This one step drive provides an accurate, repeatable readout resolution 20 times better than that used on commercial attenuators.

**12902.** Swartzendruber, L. J., Bennett, L. H., **Retained austenite developed during surface grinding of a carbon steel**, *Scr. Met.* 6, 737-742 (Aug. 1972).

Key words: Electron conversion; Mössbauer; retained austenite; standard sample; steel.

Light surface grinding on a spheroidized Fe-C alloy of the eutectoid composition raises the surface layer to a temperature sufficient to dissolve the carbide particles. The rapid quenching provided by the sample substrate and the cutting fluid retains a surface layer of austenite approximately 0.01  $\mu\text{m}$  thick. Mössbauer scattering experiments, using electron conversion, can detect the retained austenite.

**12903.** Hyman, A., Perloff, A., **The crystal structure of bismuth (2:1) borate**,  $2\text{Bi}_2\text{O}_3 \cdot \text{B}_2\text{O}_3$ , *Acta Crystallogr. B* 28, Part 7, 2007-2011 (1972).

Key words: Bismuth; borate; x-ray crystal structure.

The crystal structure of bismuth (2:1) borate ( $2\text{Bi}_2\text{O}_3 \cdot \text{B}_2\text{O}_3$ ) was determined by single-crystal x-ray diffraction analysis. Proper classification of this compound is as an oxide-orthoborate with the formula  $\text{Bi}_4\text{O}_3(\text{BO}_3)_2$ . The material crystallizes in the monoclinic system,  $P2_1/c$ , with 4 formula units in a cell of dimensions  $a = 11.107$ ,  $b = 6.627$ ,  $c = 11.044$  Å and  $\beta = 91.04^\circ$ . Intensity data were obtained on an automated diffractometer using Nb-filtered Mo  $K\alpha$  radiation ( $\lambda = 0.71069$  Å). Bismuth positions were established by direct phase determining procedures and the remaining atomic positions found from a three-dimensional difference synthesis phased by the bismuth atoms. Full-matrix, least-squares, isotropic refinement of the structure yielded a residual  $R = 5.1\%$  for 2098 observed reflections. The structure contains discrete planar  $\text{BO}_3^{3-}$  anions held together by coordination to bismuth atoms. Additional oxygen atoms, coordinated only to bismuth, are present. The average B—O distance is 1.38 Å. The minimum Bi—O distance found is 2.14 Å. Some of the bismuth atoms do not have a clearly delineated coordination shell.

12904. Perloff, A., **The crystal structures of hydrated calcium and ammonium monofluorophosphates:  $\text{CaPO}_3\text{F} \cdot 2\text{H}_2\text{O}$  and  $(\text{NH}_4)_2\text{PO}_3\text{F} \cdot \text{H}_2\text{O}$** , *Acta Crystallogr.* B28, Part 7, 2183-2191 (1972).

Key words: Ammonium fluorophosphate monohydrate; calcium fluorophosphate dihydrate; crystal structure; fluorophosphate ion.

With the primary intention of establishing the dimensions and configuration of the monofluorophosphate ion, the crystal structures of the calcium and ammonium salts have been determined by three-dimensional x-ray diffraction analysis. Data were measured on an automated diffractometer using Nb-filtered Mo  $K\alpha$  radiation,  $\lambda = 0.71069 \text{ \AA}$ . Both structures were established by direct phase determining techniques and refined by full-matrix least-squares analysis using anisotropic thermal parameters for the nonhydrogen atoms and isotropic thermal parameters for the hydrogen atoms. All hydrogen atoms were located in difference maps and the hydrogen bonding in these structures could be unambiguously determined. The crystal data (at  $25^\circ\text{C}$ ) and final  $R$  values are:  $\text{CaPO}_3\text{F} \cdot 2\text{H}_2\text{O}$ ;  $P\bar{1}$ ,  $a = 8.6497$  (7),  $b = 6.4614$  (6),  $c = 5.7353$  (4)  $\text{\AA}$ ,  $\alpha = 119.003$  (7),  $\beta = 110.853$  (7),  $\gamma = 94.146$  (8)°,  $V = 249.94 \text{ \AA}^3$ ,  $Z = 2$ ,  $\rho_c = 2.313 \text{ g.cm}^{-3}$ ,  $R = 2.0\%$  (1254 observed data).  $(\text{NH}_4)_2\text{PO}_3\text{F} \cdot \text{H}_2\text{O}$ ;  $P2_1/c$ ,  $a = 6.3042$  (5),  $b = 8.2942$  (7),  $c = 12.7597$  (10)  $\text{\AA}$ ,  $\beta = 98.415$  (8)°  $V = 660.00 \text{ \AA}^3$ ,  $Z = 4$ ,  $\rho_c = 1.530 \text{ g.cm}^{-3}$ ,  $R = 3.6\%$  (1721 observed data). The average dimensions of the  $\text{PO}_3\text{F}^{2-}$  ion are:  $\text{P} - \text{F} 1.585$ ,  $\text{P} - \text{O} 1.506 \text{ \AA}$ ,  $\text{F} - \text{P} - \text{O} 104.5$  and  $\text{O} - \text{P} - \text{O} 114.0^\circ$ .

12905. Cezairliyan, A., **Measurement of melting point and electrical resistivity (above 3600 K) of tungsten by a pulse heating method**, *High Temp. Sci.* 4, No. 3, 248-252 (June 1972).

Key words: Electrical resistivity; high-speed measurements; high temperature; melting point; thermodynamics; tungsten.

A subsecond duration pulse heating method is used to measure the melting point, and electrical resistivity of tungsten above 3600 K. The results yield a value of 3695 K (on the International Practical Temperature Scale of 1968) for the melting point with an estimated inaccuracy of 15 K. Estimated inaccuracy in electrical resistivity measurements is 1%.

12906. Rubin, R. J., **Velocity autocorrelation function of a large cluster of particles in a one-dimensional crystal**, *J. Chem. Phys.* 57, No. 1, 312-316 (July 1, 1972).

Key words: Diffusion coefficient; harmonic crystal; velocity autocorrelation function.

The velocity autocorrelation function of the center of gravity of a cluster of  $Q$  particles in a one-dimensional harmonic crystal is determined in the limit  $Q \rightarrow \infty$ . In this limit, the autocorrelation decreases linearly from one to zero. In the continuum limit of the lattice equations of motion the same linear form is obtained for the velocity autocorrelation function. The coefficient of self-diffusion of the cluster of  $Q$  particles equals  $kT$ , a result which is exact and independent of cluster size.

12907. Vidal, C. R., Hessel, M. M., **Heat-pipe oven for homogeneous mixtures of saturated and unsaturated vapors; application to NaLi**, *J. Appl. Phys.* 43, No. 6, 2776-2780 (June 1972).

Key words: Heat-pipe oven; laser induced resonance fluorescence; NaLi molecule; vapor mixtures.

A heat-pipe oven has been developed to produce homogeneous mixtures of a saturated vapor with an unsaturated vapor at any arbitrary well-defined ratio. The oven is able to handle materials of widely different vapor pressures and the zone containing the homogeneous vapor mixture can be made to extend

over any desired path length. With this heat-pipe oven containing sodium and lithium, the laser- and collision-induced fluorescence spectrum of the NaLi molecule has been used to study the operation of the oven. The first observation of a "propensity rule" for a polar molecule (the  $\Delta J = +1$  collision-induced NaLi line is stronger than the corresponding  $\Delta J = -1$  or 0 line) is reported.

12908. Paule, R. C., **Low level calibration mixtures for gaseous pollutants**, *Anal. Chem.* 44, No. 8, 1537-1539 (July 1972).

Key words: Air pollution standards; calibration mixtures (of gases); microbubbles; microstandards; NO;  $\text{SO}_2$ .

Low level  $\text{SO}_2$  calibration mixtures have been produced using a technique of mixing known weight  $\text{SO}_2$  microbubbles with a diluent gas. Procedures used in the production and measurement of the microbubbles of pure pollutant and in the subsequent on-the-spot dilution of the microbubbles are described. A necessary and effective passivation procedure for the dilution cylinder is given, along with a discussion of other factors that can affect the standard.

12909. Rubin, R. J., **Span of a polymer chain**, *J. Chem. Phys.* 56, No. 12, 5747-5757 (June 15, 1972).

Key words: Chain polymer; degenerate Dvoretzky-Erdős problem; lattice model; random walk.

The  $x$  span of a polymer chain is defined as the difference between the largest  $x$  coordinate and the smallest  $x$  coordinate of any segments in the chain. The polymer chain is represented by a nearest-neighbor lattice-model random walk in which the mean square displacement of each component of a single step is  $1/3$ . The distribution function of the  $x$  span of an  $N$  step random walk is obtained; and the following asymptotic formulas are obtained for its first and second moments, respectively,  $2(2N/3\pi)^{1/2}$  and  $4 \ln 2 N/3$ . The corresponding moments of the magnitude of the  $x$  component of the end-to-end distance are  $(2N/3\pi)^{1/2}$  and  $N/3$ . Excluded volume effects are not considered. It is noted that the problem of calculating the first moment of the  $x$  span is identical with the one-dimensional case of the Dvoretzky-Erdős problem, namely, the calculation of the average number of different lattice sites visited in an  $N$ -step random walk on a  $d$ -dimensional lattice.

12910. Jones, M. C., Palmer, D. C., Tien, C. L., **Infrared absorptivities of transition metals at room and liquid-helium temperatures**, *J. Opt. Soc. Amer.* 62, No. 3, 353-360 (Mar. 1972).

Key words: Absorption; chromium; iron; mirror; nickel; platinum; reflection.

Experimental data are presented for the normal spectral absorptivities of the transition metals, nickel, iron, platinum, and chromium at both room and liquid-helium temperatures in the wavelength range  $2.5\text{-}50 \text{ }\mu\text{m}$ . The absorptivities were derived from reflectivity measurements made relative to a room-temperature vapor-deposited gold reference mirror. The absorptivity of the gold reference mirror was measured calorimetrically, by use of infrared laser sources. Investigation of various methods of sample-surface preparation resulted in the choice of a vacuum-annealing process as the final stage. The experimental results are discussed on the basis of the anomalous-skin-effect theory modified for multiple conduction bands. As predicted, the results approach a single-band model towards the longer wavelengths. Agreement between theory and experiment is considerably improved by taking into account the modification of the relaxation time due to the photon-electron-phonon interaction proposed by Holstein and Gurzhi; but, particularly at helium temperatures, the calculated curve is consistently below the experimental results.



**12911.** Greenspan, M., **Acoustic transmission line; Some impedance properties**, *J. Acoust. Soc. Amer. Letters to Editor* **52**, No. 1, Part 2, 455-457 (July 1972).

Key words: Acoustic impedance; acoustic transmission line; sound absorption.

The imaginary part of the effective density of a fluid or of a viscoelastic material is zero. The contrary notion arises from an inadequate definition of characteristic impedance. The attenuation cannot exceed  $2\pi N_p$  per wavelength.

**12912.** Smith, R. V., **Two-phase, two-component critical flow in a venturi**, *J. Basic Eng. Trans. ASME, Series D* **94**, No. 1, 147-155 (Mar. 1972).

Key words: Critical flow; droplet flow; liquid film flow; transport coefficients; two-component flow; two-phase flow; venturi flow.

This paper reports the results of an analytical and experimental investigation whose object was to test the hypothesis that the flow of the gas phase controls critical and near critical two-phase flow for cases where the gas flow is essentially in separate streams. The results substantiate the hypothesis. The analytical results also indicate that one-dimensional flow equations with reasonably accurate estimates for the droplet size and for the drag and heat transfer coefficients will adequately describe critical and near critical flow over a wide range of flow conditions.

**12913.** Patrician, T. J., Ledbetter, H. M., Reed, R. P., **On the apparent rotation of transformation twins in Fe-Ni martensites**, *Metallurgical Trans.* **3**, No. 4, 947-952 (Apr. 1972).

Key words: Crystal imperfections; electron diffraction crystallography; iron alloys; nickel alloys; phase transformations/solid-state; twinning.

Fe-Ni alloys containing 28 to 33 wt pct Ni have been studied by transmission electron microscopy and by selected area diffraction to elucidate the phenomenon of the apparent deviation of the twin interface from the twinning plane  $\{112\}_m$ . Trace analyses of the twin interfaces are reported for 35 cases. Deviations of the twin trace, as projected onto the image plane, of up to 46 deg from those expected from  $\{122\}_m$  transformation twins were observed. Contrary to previous interpretations, the conclusion of this study is that the deviations are due to the uncertainty of the orientation of the foil surface with respect to the electron beam. Thus, it has not been shown explicitly that this phenomenon provides a basis either for invoking multiple lattice invariant shears or for explaining habit plane scatter.

**12914.** Dickens, B., Bowen, J. S., Brown, W. E., **A refinement of the crystal structure of  $\text{CaHPO}_4$  (synthetic monetite)**, *Acta Crystallogr.* **B28**, Part 3, 797-806 (Mar. 1972).

Key words: Calcium coordinations; calcium phosphates; hydrogen bonding; monetite single crystals; x-ray diffraction.

$\text{CaHPO}_4$ , synthetic monetite, crystallizes in the triclinic unit cell  $a = 6.910$  (1),  $b = 6.627$  (2),  $c = 6.998$  (2) Å,  $\alpha = 96.34$  (2)°,  $\beta = 103.82$  (2)°,  $\gamma = 88.33$  (2)° at 25 °C with cell contents of  $4[\text{CaHPO}_4]$ . The structure has been refined in space-group  $P\bar{1}$  by the method of least-squares to  $R_w = 0.032$ ,  $R = 0.031$  using 3738 observed x-ray reflections measured on a diffractometer. Corrections were made for absorption, anomalous dispersion and isotropic secondary extinction.

The structure may be considered to consist of  $\text{CaHPO}_4$  chains bonded together by  $\text{Ca}\dots\text{O}$  bonds and three types of hydrogen bonds. One type of hydrogen bond,  $\text{O}(1) - \text{H}(1)\dots\text{O}(5)$ , is normal but is at the short end of the normal range with  $\text{O}(1)\dots\text{O}(5) = 2.565$  (1) Å; one,  $\text{O}(7) - \text{H}(2)\dots\text{O}(7')$ , is very short with

$\text{O}(7)\dots\text{O}(7') = 2.458$  (2) Å and is across a nominal center of symmetry; and one,  $\text{O}(6) - \text{H}(3)\dots\text{O}(8)$  where  $\text{O}(6)\dots\text{O}(8) = 2.669$  (1) Å, is in the normal range but is presumed to be statistically disordered, with hydrogen covalently bonded to half of the  $\text{O}(6)$  atoms on average. The  $P - O$  distances support the choice of these hydrogen positions.  $\text{Ca}(1)$  is coordinated to seven oxygen atoms in an approximately pentagonal bipyramid with  $\text{Ca}(1)\dots\text{O}$  distances ranging from 2.2951 (9) Å to 2.763 (1) Å.  $\text{Ca}(2)$  is coordinated to eight oxygen atoms with  $\text{Ca}(2)\dots\text{O}$  distances ranging from 2.379 (1) Å to 2.5718 (9) Å, which all indicate strong  $\text{Ca}\dots\text{O}$  bonding. The Ca coordinations in several calcium phosphates and related compounds are compared.

**12915.** Bowen, R. L., Argentar, H., **A stabilizing comonomer: I. Synthesis and confirmation of structure**, *J. Dent. Res.* **51**, No. 4, 1071-1074 (July-Aug. 1972).

Key words: Antioxidants; biomaterials; comonomers; inhibitors; polymerization; stabilizers; toxicity.

A compound (BHM) was synthesized that can stabilize monomers by inhibiting premature polymerization but that can serve as a monomer in the polymerization after the initiator system is activated. The structural formula of BHM (3,5-di-*tert*-butyl-4-hydroxybenzyl methacrylate) was confirmed by nuclear magnetic resonance analysis.

**12916.** Paffenbarger, G. C., **Guide to Dental Materials and Devices: a historical review**, *J. Amer. Dent. Ass.* **84**, 1333-1335 (June 1972).

Key words: Certification program; guide; list of certified dental materials; specifications; Wilmer Souder.

The Guide to Dental Materials and Devices is a biennial publication of the American Dental Association. It started in 1955 as a publication of the ADA Specifications for Dental Materials. Dr. Wilmer Souder, a physicist who was the founder and former chief of the Dental Research Section, National Bureau of Standards, originated the idea and gave the motivation for the original specification for dental materials and the subsequent Guide. The Guide is not intended to replace dental materials textbooks, but is a source of current information for dentists, assistants and dental prosthetic laboratory technicians to guide them in their selection and use of dental materials. The Sixth Edition 1972-1973 will be published in May or June of this year. It is a professional book with extensive references and is prepared by a professional society for its members and their auxiliaries.

**12917.** Mihalas, D., Hummer, D. G., Conti, P. S., **On the N III  $\lambda\lambda 4640, 4097$  lines in Of stars**, *Astrophys. J.* **175**, No. 2, Part 2, L99-L104 (July 15, 1972).

Key words: Dielectronic recombination; ionized nitrogen; Of stars; stellar atmospheres; stellar spectra.

Detailed calculations based on non-LTE plane-parallel model atmospheres show that the N III emission lines at  $\lambda\lambda 4634, 4640, 4641$  observed in Of stars are produced primarily by dielectronic recombination to  $3d^3D$  followed by the  $3d^3P$  transition in a compact atmosphere. The  $3p$  state in turn is drained by two-electron transitions to the  $2p^2$  levels. We find that  $\lambda 4640$  is in emission for  $T_{\text{eff}} \leq 37,000$  K for main-sequence objects (33,000 K for giants), while  $\lambda 4097$  remains strongly in absorption, in accordance with observations. The calculated equivalent widths are in substantial agreement with the observed values for those Of stars with He II  $\lambda 4686$  in absorption, i.e., for those objects designated by Walborn as O(f).

**12918.** Peterson, R. L., **Pseudoresonances in the magnetophonon structure of nondegenerate semiconductors**, *Phys. Rev. Lett.* **28**, No. 7, 431-434 (Feb. 14, 1972).

Key words: Boltzmann equation; magnetophonon effect; semiconductors; transport theory.

A new oscillatory behavior of semiconductor transport properties in quantizing magnetic fields is predicted on general arguments. The "pseudoresonances" are due to the pairing off of single-LO-phonon emission and absorption processes ending at the infinite density-of-states region. An exact calculation of Ohmic longitudinal magnetoresistance shows that at "high" temperatures, the pseudoresonance amplitudes are comparable to the usual magnetophonon resonances. The pseudoresonances have probably been seen, but attributed to 2LO-phonon scattering processes.

**12919.** Young, R., Ward, J., Scire, F., **The topografiner: An instrument for measuring surface microtopography**, *Rev. Sci. Instrum.* **43**, No. 7, 999-1011 (July 1972).

Key words: Diffraction grating; field emission; micrometrology; profile; surface; surface instrumentation; surface metrology; topography; tunneling.

A noncontacting instrument for measuring the microtopography of metallic surfaces has been developed to the point where the feasibility of constructing a prototype instrument has been demonstrated. The resolution of the preprototype unit is 30 Å perpendicular to the surface and 4000 Å in the plane of the surface. Inherent noise in the perpendicular direction corresponds to 3 Å or one atomic layer. By using a typical field emitter with radius of 100 Å, an ultimate limit of 200 Å would be expected for the horizontal resolution. Topographic maps of an infrared diffraction grating have been measured in order to demonstrate the performance of the instrument in measuring a well characterized surface. The instrument has been shown to conform to the Fowler-Nordheim description of field emission while spaced at the usual operating distances from the surface. When moved to within 30 Å of the surface, its performance is compatible with Simmons' theory of MVM tunneling. In the MVM mode, the instrument is capable of performing a noncontacting measurement of the position of a surface to within about 3 Å. The instrument can be used in surface science experiments to study the density of single and multiple atom steps on single crystal surfaces, adsorption of gases, and processes involving electronic excitations at surfaces.

**12920.** Opal, C. B., Beaty, E. C., Peterson, W. K., **Tables of secondary-electron-production cross sections**, *At. Data* **4**, No. 3, 209-253 (July 1972).

Key words: Atmospheric gases; cross section measurement; noble gases; secondary electrons.

The normalized results of relative measurements of electron-production cross sections differential in angle over the 30 to 150° range and in ejected energy over the 4 to 200 eV range are tabulated. Primary electron energies from 50 to 2000 eV were used in the study of He, N<sub>2</sub>, and O<sub>2</sub>. The remaining gases (Ne, Ar, Kr, Xe, H<sub>2</sub>, CH<sub>4</sub>, NH<sub>3</sub>, H<sub>2</sub>O, CO, C<sub>2</sub>H<sub>2</sub>, NO, and CO<sub>2</sub>) were studied under 500 eV impact. Measurements were performed in a crossed-beam apparatus with the use of a rotatable electron gun and a fixed hemispherical electrostatic energy analyzer.

**12921.** Dickens, B., Bowen, J. S., **Refinement of the crystal structure of Ca(H<sub>2</sub>PO<sub>4</sub>)<sub>2</sub> · H<sub>2</sub>O**, *Acta Crystallogr.* **B27**, Part 11, 2247-2255 (Nov. 1971).

Key words: Calcium phosphates; crystal structure; hydrated calcium phosphate; hydrogen bonding; monocalcium phosphate monohydrate; single crystal x-ray diffraction.

Ca(H<sub>2</sub>PO<sub>4</sub>)<sub>2</sub> · H<sub>2</sub>O crystallizes in space group *P* $\bar{1}$  in the triclinic unit cell  $a = 5.6261$  (5),  $b = 11.889$  (2),  $c = 6.4731$  (8) Å,  $\alpha = 98.633$  (6),  $\beta = 118.262$  (6), and  $\gamma = 83.344$  (6)° at 25 °C with

$Z = 2$ . The structure was refined with 3401 observed reflections measured on a diffractometer to  $R_w = 0.033$ ,  $R_o = 0.069$ . Corrections were made for absorption, anomalous dispersion, and isotropic secondary extinction. The structure contains Ca(H<sub>2</sub>PO<sub>4</sub>)<sup>+</sup> chains which form corrugated layers. Between these layers are layers of (H<sub>2</sub>PO<sub>4</sub>)<sup>-</sup> ions and water molecules. Hydrogen atoms have been located approximately; ideal positions for the hydrogen atoms have been calculated. The two sets of hydrogen positions differ by  $\sim 0.28$  Å. One hydrogen bond, in which the water molecule is the donor, is apparently bifurcated. All other hydrogen atoms form normal hydrogen bonds, with each hydrogen site seemingly fully occupied. The disorder of one hydrogen atom between the centrosymmetrically related atoms O(1) and O(1') was postulated by earlier workers. The P—O and O...O distances and electron-density maps obtained here show that there is no hydrogen atom in this position.

**12922.** Bowen, R. L., Argentar, H., **Tertiary aromatic amine accelerators with molecular weights above 400**, *J. Dent. Res.* **51**, No. 2, 473-482 (Mar.-Apr. 1972).

Key words: Accelerators; amines; color-stable composites; crystalline amine polymerization accelerators; synthesis; toxicity.

With the proper ring substituents, tertiary aromatic amines with large substituents on the nitrogen atom can be effective accelerators in free radical polymerization. Resistance to discoloration appears to be primarily a function of the substituents on the aromatic ring of the amine, whereas the rate of polymerization is dependent on both the alkyl substituents on the ring and the groups attached to the nitrogen atom.

**12923.** Brauer, G. M., Huget, E. F., **Dental adhesives**, Chapter 16 in *The Chemistry of Biosurfaces*, M. L. Hair, ed., **2**, 731-800 (Marcel Dekker, New York, N.Y., 1972).

Key words: Adhesives; adhesive test methods; bioadhesives; dental adhesives; dental resins; reactivity of tooth surfaces; tooth surface treatments.

Reactions occurring at the tooth surfaces and methods for obtaining bonding of restorative resins to enamel and dentin are reviewed. The composition of the tooth structure and the physical and mechanical properties of enamel and dentin are given. Studies of the reactivity of tooth surfaces as determined from adsorption, heats of immersion and wettability measurements are discussed. The effectiveness of various surface treatments such as by etching agents, enzymes, coupling agents and surface grafting techniques are examined. The potential organic polymeric adhesive systems, including bioadhesives useful for dental applications, are summarized. Methods of testing the magnitude of the adhesive joint are described.

**12924.** Jefferies, J. T., Orrall, F. Q., Zirker, J. B., **The interpretation of total line intensities from optically thin gases. I. A general method**, *Solar Phys.* **22**, No. 2, 307-316 (Feb. 1972).

Key words: Optically thin line emission; radiative transfer; solar corona; spectroscopic diagnostics.

We describe a general method for inferring, from the line emission of an optically thin medium, the physical state of the gas along the column in the line of sight which is sampled by the observations. Since it is not possible to infer the distribution of the physical state parameters with position in the line of sight—any arbitrary rearrangement of material giving equivalent line emission—we seek instead to specify the state in another way. A unique specification is found in terms of the bivariate distribution function  $\mu(n, T)$ , describing the partitioning of the matter in the gas over the density and temperature. We show that, given sufficient observational data, it is in principle possible to determine



both  $\mu(n, T)$ , and the chemical composition. With less complete data the acuity of the analysis is correspondingly reduced.

The method is devised for application to the astronomical case, especially for studies of the solar corona, the chromosphere-corona transition region, planetary nebulae and other optically thin sources. We illustrate the formulation for the situation encountered in the solar corona.

**12925.** Jefferies, J. T., Orrall, F. Q., Zirker, J. B., **The interpretation of total line intensities from optically thin gases. II. The coronal forbidden lines**, *Solar Phys.* 22, No. 2, 317-326 (Feb. 1972).

Key words: Optically thin line emission; radiative transfer; solar corona; spectroscopic diagnostics.

We discuss the application of a general diagnostic procedure, developed in the preceding paper of this series, to the inference of the physical state of coronal condensations from a knowledge of their forbidden line emission. We consider the limitations set on such an analysis by inadequacies in existing data and indicate the additional observations in the infrared and ultraviolet, as well as the visible, which will be needed for development of the full power of the diagnostic method.

**12926.** Jefferies, J. T., Orrall, F. Q., Zirker, J. B., **The interpretation of total line intensities from optically thin gases. III. Application to coronal forbidden line spectra**, *Solar Phys.* 22, No. 2, 327-343 (Feb. 1972).

Key words: Optically thin line emission; radiative transfer; solar corona; spectroscopic diagnostics.

The diagnostic method developed in the two preceding papers of this series is applied to coronal forbidden line intensity data obtained at eclipses in 1952, 1961, 1965, 1966, and 1970. The application of the method is limited by the nature of the data but allows a first inference of the relationship between electron density and temperature in the condensations observed at these eclipses, and of the distribution of the electrons within the temperature range samples by the observations—effectively  $10^6$  to  $2.4 \times 10^6$  K. We determine the relative abundance of nickel to iron in the corona, finding a value in agreement with latest photospheric determinations and with a similar (factor of two) uncertainty. We are also able to set lower limits to the abundance of iron with respect to hydrogen, again finding values consistent with recent photospheric determinations.

**12927.** Lightbody, J. W., Jr., **Electron scattering from one- and two-phonon vibrational states**, *Phys. Lett.* 38B, No. 7, 475-479 (Apr. 3, 1972).

Key words: Admixture; anharmonicities; branching ratios; electron scattering; phonons; reorientation effect.

Admixtures of one- and two-phonon states are required to fit (e, e') form factors for the lowest two  $2^+$  states in several even-even vibrational nuclei. These anharmonic wave functions correctly reproduce radiative branching ratios and excited state quadrupole moments.

**12928.** Neuhausen, R., Lightbody, J. W., Jr., Fivozinsky, S. P., Penner, S., **Elastic electron scattering from Zn isotopes**, *Phys. Rev. C* 5, No. 1, 124-128 (Jan. 1972).

Key words: Electron scattering; nuclear radii; nuclear sizes; zinc nuclei.

Elastic electron scattering from the stable even-even Zn isotopes was measured in the region of the first diffraction minimum ( $0.3 \leq q \leq 1.1 \text{ fm}^{-1}$ ). The cross-section ratios for each pair of isotopes were used to determine the change in the rms radius. The rms radius follows an  $A^{1/3}$  law between  $^{64}\text{Zn}$  and  $^{66}\text{Zn}$

and between  $^{68}\text{Zn}$  and  $^{70}\text{Zn}$ ; whereas, between  $^{66}\text{Zn}$  and  $^{68}\text{Zn}$  the rms radius decreases significantly.

**12929.** Bergstrom, J. C., Crannell, H., Kline, F. J., O'Brien, J. T., Lightbody, J. W., Jr., Fivozinsky, S. P., **Electroexcitation of the giant resonance of  $^{13}\text{C}$** , *Phys. Rev. C* 4, No. 5, 1514-1532 (Nov. 1971).

Key words: Continuum spectra; efficiencies; fine structure; giant resonance; isospin splitting; pygmy; pygmy resonance; radiative tails; resonance weak coupling;  $^{12}\text{C}$ ,  $^{13}\text{C}$ .

The giant resonance of  $^{13}\text{C}$  has been investigated by means of inelastic electron scattering. The incident energies and scattering angles employed were 77.0 MeV ( $75^\circ$ ), 106.0 MeV ( $75^\circ$ ), 55.4 MeV ( $145.7^\circ$ ), and 81.0 MeV ( $145.7^\circ$ ). The data show a distinct splitting of the resonance into two large peaks near 20.5 and 24.5 MeV. Some fine structure is observed which correlates well with the position of excitations calculated by Easlea. Considerable strength is observed in the region of 14-MeV excitation which may correspond to the "pygmy" resonance seen in the photonuclear work of Cook. Data were also taken consecutively on  $^{12}\text{C}$ . The form factors for  $^{12}\text{C}$  and  $^{13}\text{C}$  are compared. The presence of the extra neutron in  $^{13}\text{C}$  results in a major restructuring of the giant-resonance strength. The possibility of an isotopic splitting in the  $^{13}\text{C}$  giant resonance is discussed.

**12930.** Pruitt, J. S., **Electron beam current monitoring system II**, *Nucl. Instrum. Methods* 100, 433-443 (1972).

Key words: Beam; calibration electron; Faraday-cup; ferrite; monitor.

A reliable method for absolute calibration of a ferrite electron beam current monitor with a pulse generator has been developed and tested. The absolute accuracy of pulser calibrations and Faraday cup calibrations of the National Bureau of Standards ferrite monitor has been compared by using them both to determine the Faraday cup error. These independent determinations differ by a maximum of 0.11% and an average of 0.03% at six different energies in the 20-120 MeV range, using beam currents between 0.6 and 25  $\mu\text{A}$ . Variation of the Faraday cup error with energy is shown to compare favorably with the predictions of other authors, and the good agreement is used to argue that the influence of beam microstructure on the ferrite calibration is less than 0.1%.

**12931.** Becker, D. A., **Trace analysis for platinum in glasses by neutron activation**, *Anal. Chim. Acta* 61, 1-6 (1972).

Key words: Glasses; neutron activation analysis; radiochemical separations; spontaneous deposition; trace analysis.

Trace amounts of platinum were determined in eight glasses. These glasses had been prepared under special conditions, and information on both the surface and interior platinum was desired. Previous microscopic examination of the glass samples had identified platinum on the surface of at least four of the samples. The platinum was analyzed using the nuclear reaction  $^{198}\text{Pt}(n, \gamma)^{199}\text{Pt} \xrightarrow{\beta^-} ^{199}\text{Au}$ . The  $^{199}\text{Au}$  product has a 3.15 day  $T_{1/2}$  and  $E_\gamma$  of 158 and 208 keV. Samples were irradiated in the NBSR for 2 hours at  $1.3 \times 10^{13} \text{ n} \cdot \text{cm}^{-2} \text{ sec}^{-1}$ . After irradiation, the glasses were etched with aqua regia for the determination of surface platinum, and then dissolved in HF and  $\text{HClO}_4$  for the determination of interior platinum. The radioactive  $^{199}\text{Au}$  was separated from the matrix by spontaneous deposition on metallic zinc. Experimental sensitivities of 0.02  $\mu\text{g}$  platinum were obtained.

**12932.** Pringle, W. C., Jr., **Microwave spectrum, vibration-rotation interaction, and ring puckering vibration in silacyclobutane**

and silacyclobutane-1,1- $d_2$ , *J. Chem. Phys.* **54**, No. 12, 4979-4988 (June 15, 1971).

**Key words:** Dipole moment; molecular structure; ring puckering vibration; rotational spectrum; silacyclobutane; vibrational potential functions; vibration-rotation interaction.

The microwave spectrum of the molecules silacyclobutane and silacyclobutane-1, 1- $d_2$  has been observed between 8 and 55 GHz and the first four vibrational states assigned. The ground state rotational constants of the former molecule are 8815.75, 6289.00, and 4245.32 MHz. The first two inversionlike intervals of the ring puckering mode were determined to be 75.75 and 7790 MHz in the normal isotopic species; the corresponding intervals in the deuterated species are 43.06 and 4430 MHz. The effect of these frequencies on the determination of the potential energy for the ring puckering vibration was investigated. The ring configuration was shown to be significantly puckered in the ground state. The  $a$  component of the dipole moment was found to be nearly constant in the four vibrational states of the normal molecule,  $\mu_a = 0.4396$  D, while the out-of-plane transition moment between inversion doublets dropped rapidly as the inversion levels approached the top of the barrier.

**12933.** Peterson, R. L., **Longitudinal magnetoresistance in polar semiconductors: A displaced-Maxwellian analysis**, *Phys. Rev. B* **5**, No. 10, 3994-4000 (May 15, 1972).

**Key words:** InSb; magnetophonon; magnetoresistance; semiconductors; transport theory.

The displaced-Maxwellian distribution function is used to study longitudinal magnetoresistance in polar semiconductors, when several carrier scattering mechanisms are simultaneously active. Although both the  $B=0$  and the quantum-limit expressions for the resistance are largely the same as those obtained from the Boltzmann equation, numerical calculations show that the displaced Maxwellian is unable to account for longitudinal magnetoresistance minima often observed in the magnetophonon structure of polar materials. In the hot-electron regime, the displaced Maxwellian can give maxima or minima, depending upon lattice temperature and type of scattering mechanisms.

**12934.** Wiese, W. L., Kelleher, D. E., Paquette, D. R., **Detailed study of the Stark broadening of Balmer lines in a high-density plasma**, *Phys. Rev. A* **6**, No. 3, 1132-1153 (Sept. 1972).

**Key words:** Asymmetries; hydrogen lines; line profiles; shifts; stabilized arc; Stark broadening.

The Stark-broadened profiles of the Balmer lines  $H_\alpha$ ,  $H_\beta$ ,  $H_\gamma$ , and  $H_\delta$  have been measured in a high-current, wall-stabilized arc operated in hydrogen. Temperatures and electron densities have been determined with a plasma model assuming partial local thermodynamic equilibrium (LTE), after a detailed plasma analysis revealed small deviations from complete LTE. The temperatures have been determined from line-to-continuum intensity ratios using  $H_\beta$  and continuum points in the near uv, and the electron densities were derived from absolute intensity measurements. The investigations cover the range of electron densities between  $1.5 \times 10^{16}$  and  $10^{17}$  cm $^{-3}$  and temperatures between  $0.9 \times 10^4$  and  $1.4 \times 10^4$  K. Extensive comparisons with recent Stark-broadening theories and other experiments have been undertaken with the following principal results: The most pronounced differences between this experiment and theory occur in and near the line centers, where the measured profiles show systematically less structure than the calculations predict. Comparisons of the calculated and precisely measured ratios between the 1/2, 1/4, and 1/8 widths within each line show that the recent theories are internally consistent within 6% for  $H_\beta$  and  $H_\gamma$ , whereas for  $H_\alpha$  inconsistencies of order 25% occur. Similar

inconsistencies, somewhat larger respectively, are found for the theoretical values of the half-width ratios between different Balmer lines. For the most important line  $H_\beta$ , the measured half-widths agree within 7% with the calculated values. The total experimental error in this comparison, which originates predominantly in the electron-density measurement, is estimated not to exceed 6%. Very reproducible asymmetries and red shifts are observed for  $H_\beta$  and  $H_\gamma$ . Somewhat smaller red shifts are also obtained for  $H_\alpha$ . The shifts are approximately linear functions of the electron density. Comparisons with other experimental data show appreciable scatter between the various results. We estimate that for the most-often-studied line  $H_\beta$  the uncertainties in the theoretical Stark widths are of the order of (5-7)% for the range of our experiment.

**12935.** Moore, G. A., **Automatic methods for analysis of microstructures**, (American Society for Testing and Materials Symp. on Stereology and Quantitative Metallography, Atlantic City, N.J., June 28, 1971), *Amer. Soc. Test. Mater. Spec. Tech. Publ.* **504**, pp. 59-80 (July 1972).

**Key words:** Aggregates; anisotropy; automation; computers; mechanical properties; microscopes; microstructure; particle distribution; phase mapping; quality control; scanning; television systems; variability; variance (statistics).

From the viewpoint of materials engineering and quality control the significant aspects of the microstructure of a material as a whole constitute a gestalt which controls mechanical behavior. This gestalt can be specified by six stereologically valid parameters measuring phase percentage, size and spacing of particles, variability among portions of the material, general anisotropy, and degree of patternness. Raster scanning devices of either the mechanical or television type are intrinsically capable of easily measuring these six parameters. Provision for each is available in at least one of the present television scanners. Minor changes are desirable to provide this common set of measurements with all instruments and to improve accuracy.

In contrast, microarchitectural processes which identify, measure, and selectively count individual object sections require massive programming effort and are inefficient and time consuming in present computers. Selective specimen preparation and human designation of objects are preferable to machine identification. Some proposals for more efficient and more human-like machines are mentioned. Materials engineers should try to avoid these difficult processes whenever feasible.

**12936.** Curl, R. F., Jr., Evenson, K. M., Wells, J. S., **Laser magnetic resonance spectrum of NO $_2$  at 337  $\mu$ m and 311  $\mu$ m**, *J. Chem. Phys.* **56**, No. 10, 5143-5151 (May 15, 1972).

**Key words:** HCN laser; laser magnetic resonance; NO $_2$ ; spectroscopy.

The Zeeman components of several rotational transitions of nitrogen dioxide have been observed in absorption using the 311 and 337  $\mu$ m lines of an HCN laser as a source. The Zeeman components of four rotational transitions (two at 311  $\mu$ m and two at 337  $\mu$ m) have been assigned. Two components of the  $g$  tensor have been determined from the spectrum by least square fitting. The anisotropic component  $(aa)_g^{(S)}$ , obtained as  $-0.010$ , agrees well with that predicted from theory, but the isotropic component  $(0)_g^{(S)}$ , obtained as  $2.013$ , does not agree satisfactorily with theoretical prediction or with solid phase measurements both of which give  $1.9997$ . The rotational frequencies of the four transitions have also been obtained.

**12937.** Billingsley, F. P., II, Krauss, M., **Coupled multiconfigurational self-consistent-field method for atomic dipole**



**polarizabilities. I. Theory and application to carbon, *Phys. Rev. A* 6, No. 3, 855-865 (Sept. 1972).**

**Key words:** Carbon ( $^1D$ ); carbon ( $^3P$ ); carbon ( $^1S$ ); multi-configuration; static dipole polarizability; variation method.

A method for calculating static dipole polarizabilities of atoms within a multiconfigurational self-consistent-field (SCF) framework is presented. The method involves the direct solution of the multiconfigurational SCF equations of an atom in the presence of a perturbing field which is simulated by a charged particle. The use of a multiconfigurational framework allows this technique to be applied straightforwardly to any given state of both degenerate and nondegenerate atoms, and also allows the explicit introduction of correlation effects. Sample calculations are reported for the static dipole polarizabilities of the carbon atom in its  $^1S$ ,  $^1D$ , and  $^3P$  states with partial inclusion of correlation. The results are compared with those obtained from many-body perturbation theory, and other techniques. In addition, a prescription for specifying a sufficiently flexible set of polarization basis functions is described.

**12938. Jacox, M. E., Milligan, D. E., Spectrum and structure of the  $O_3^-$  and  $O_4^-$  anions isolated in an argon matrix, *Chem. Phys. Lett.* 14, No. 4, 518-521 (June 15, 1972).**

**Key words:** Charge transfer; infrared spectrum; isotopic substitution; matrix isolation;  $O^- + O_2$  reaction;  $O_3^-$  anion;  $O_4^-$  anion; structure; ultraviolet spectrum.

An absorption which appears near  $800\text{ cm}^{-1}$  upon reaction of  $O^-$  with  $O_2$  in an argon matrix has been assigned as  $\nu_3$  of  $O_3^-$ , with a valence angle of  $110 \pm 5^\circ$ , and an absorption near  $1000\text{ cm}^{-1}$  can be assigned to *trans*- $O_4^-$ .

**12939. Franklin, A. D., Defect equilibria in alkaline earth fluorides containing rare earth ions, *Tech. Rep. AFML-TR-72-31*, 48 pages (Air Force Materials Laboratory, Air Force Systems Command, Wright-Patterson Air Force Base, Ohio, Mar. 1972).**

**Key words:** Anelastic relaxation;  $CaF_2$ ; density; dielectric relaxation; EPR; equilibria; point defects; rare-earth doping.

The point defects present in  $GdF_3$ -doped  $CaF_2$ , with concentrations ranging from 0.01 to 0.46 mole percent  $GdF_3$ , have been studied using measurements of density, EPR, and dielectric and anelastic relaxation as a function of concentration and of annealing temperature in an  $He + HF$  atmosphere in the range 500 to  $1100^\circ C$ . The density measurements showed no dependence upon annealing. The unit cell contents increased in mass with increasing  $GdF_3$  concentration more rapidly than expected on the basis of substitutional  $Gd^{3+}$  and interstitial  $F^-$  ions, and suggest the incorporation of an  $HF$  molecule with each  $GdF_3$  unit. The role previously suggested for cation vacancies in the annealing behavior appears untenable in light of these density results. The reorientation kinetics of the pair formed by association of the mobile interstitial  $F^-$  ion with the immobile  $Gd^{3+}$  ion were studied using EPR line-broadening and dielectric relaxation measurements, and some anelastic relaxation measurements were made as well. The EPR line-broadening and dielectric relaxation data could be fitted very well with the same model, in which reorientation takes place in a mode dominated by nearest-neighbor jumps of the interstitial  $F^-$  ion. This jump frequency is given by  $3.1 \times 10^{12} \exp(-0.38\text{ eV/kT})\text{ s}^{-1}$ . Additional relaxation modes appear in both the dielectric and anelastic spectra, and at least 2 and perhaps 3 centers are involved, as yet unidentified.

**12940. Richmond, J. C., Kneissl, G. J., Procedures for the precise determination of thermal radiation properties, *Tech. Rep. AFML-TR-70-121*, 104 pages (Air Force Materials Laboratory,**

**Air Force Systems Command, Wright-Patterson Air Force Base, Ohio, Oct. 1970).**

**Key words:** Emittance; graphite; iridium; laser-source integrating sphere; reflectance; shallow cavity emittance; surface characterization; thoria; tungsten.

The broad objective of this program, which has continued for several years, is to develop equipment and procedures for measuring the important thermal radiation properties of materials, particularly those used in aircraft, missiles, and space vehicles, at temperatures up to the melting points of the most refractory materials. During the period covered by this report the specific objectives were to complete development of the laser-source integrating sphere reflectometer, and to prepare emittance standards for use at temperatures above  $1400\text{ K}$  ( $2000^\circ F$ ). The laser-source integrating sphere reflectometer consisted of (1) a helium-neon laser as a source, capable of operation at  $0.6328$ ,  $1.15$ , and  $3.39\text{ }\mu\text{m}$ ; (2) a  $35\text{ cm}$  ( $14\text{ in.}$ ) diameter sphere coated with barium sulphate or sodium chloride; (3) a lead sulfide detector; and (4) a radio-frequency generator for heating the sample by induction. A spike filter, transmitting at the laser-wavelength, placed in front of the detector, reflected or absorbed most of the background radiation from the hot sample, and a chopped incident beam together with synchronous amplification of the signal from the detector was used to eliminate the effect of the remaining background radiation. The integrating sphere could be evacuated, or used with an atmosphere of purified helium. An error analysis showed that the measured absolute reflectance is measured with a bias of less than one percent of the measured value. Data are presented on the directional-hemispherical reflectance  $[\rho(12^\circ; 2\pi)]$  at temperatures in the range of  $1300$  to  $2500\text{ K}$  of well characterized samples of thoria, iridium, two lots of graphite and two lots of tungsten. Precision of measurement on the order of  $0.0005$  in reflectance units, expressed as the standard deviation of six replicate measurements, was attained. Samples of one lot of tungsten and one lot of graphite were supplied by Arthur D. Little, Inc., from the same lots as those for which thermal conductivity data are reported in AFML-TR-69-2. Data are also presented for the normal total emittance of alumina, thoria, magnesia, zirconia, graphite, iridium and two lots of tungsten, obtained by the shallow cavity technique and modifications thereof, at temperatures in the range of  $1400$  to  $2500\text{ K}$  (about  $2000$  to  $4000^\circ F$ ).

**12941. Mountain, R. D., Temperature dependence of depolarized scattered light near the critical point, (Proc. of the Colloquium on Light Scattering by Fluids, Paris, France, July 15-17, 1971), *J. Phys.* 33, Supplement 2-3, C1-265 - C1-268 (Feb.-Mar. 1972).**

**Key words:** Correlation length; critical opalescence; critical phenomena; depolarized scattering; light scattering; Ornstein-Zernike correlation function.

The double scattering formalism of Frish and McKenna is used to investigate the temperature dependence of the depolarized scattering in the vicinity of the critical point of a one component fluid composed of spherical molecules. The terms involving two particle correlations are estimated using the Ornstein-Zernike correlation function. The ratio of the intensity of the  $H-H$  to  $V-V$  scattering is found to diverge as  $k\xi \ln(1/k\xi)$ . The possibility of using depolarized scattering as a probe of three and four particle correlations near the critical point is discussed.

**12942. McNesby, J. R., Braun, W., Ball, J., Vacuum ultraviolet techniques in photochemistry, Chapter 11 in *Creation and Detection of Excited State*, A. A. Lamola, ed., 1, 503-586 (Marcel Dekker, Inc., New York, N.Y., 1971).**

**Key words:** Actinometry; experimental; light sources; photochemistry; vacuum ultraviolet; window materials.



Vacuum ultraviolet techniques in photochemistry are reviewed from the standpoint of light sources (both continuously operated and pulsed), window materials, actinometry and chemical applications. Emphasis is given to modern physical techniques.

**12943.** Leasure, W. A., Jr., **Considerations in the development of measurement procedures for the regulation and monitoring of noise pollution**, (Proc. 2d Urban Technology Conf. and Technical Display, San Francisco, Calif., July 24-26, 1972), *AIAA Paper No. 72-622*, pp. 1-10 (American Institute of Aeronautics, New York, N.Y., 1972).

**Key words:** Acoustics; noise measurement; noise pollution; noise regulations; noise (sound).

A noise standard or regulation should be based on accurate, reliable and relevant measurements. In this paper, an outline is given of some of the basic considerations in developing measurement systems which are required in order to effectively regulate or monitor noise pollution or to assess the alternative strategies for noise abatement and control. The importance of these considerations is reinforced through a discussion of the questions addressed during the design of a test procedure and measurement methodology for a specific program in the area of motor vehicle noise.

**12944.** Wood, L. A., Bullman, G. W., **Creep and other tensile properties of rubber crosslinked by dicumyl peroxide**, *J. Polym. Sci.: Part A-2*, **10**, 43-50 (Jan. 1972).

**Key words:** Creep; modulus; rubber, natural; tensile properties; tensile strength; ultimate elongation.

Natural rubber crosslinked by dicumyl peroxide in amounts up to 25 parts per hundred of rubber (phr) showed a maximum in tensile strength near 1 phr, followed by a steep decrease to a minimum near 5 phr. The ultimate elongation decreased from 870% at 0.5 phr to about 10% above 10 phr. The modulus increased linearly with increase of crosslinking. The creep rate decreased from 5.6% per decade at 0.5 phr to zero at 5 phr and higher values. Crystallization, with a resultant abrupt increase in creep, was noted in specimens held in the stretched condition for more than one day. Between 5 and 25 phr this system (when crystallization is avoided) appears to function as an ideal elastic network and can be recommended for studies of rubber elasticity since no variation of modulus with time is observed.

**12945.** Miller, A., McLaughlin, W. L., Lynggard, B., **A scanning spectrophotometer for reading thin-film dosimeters**, *Dan. At. Energy Comm. Risö Rep. No. M-1525*, pp. 1-21 (Aug. 1972).

**Key words:** Dose distribution; dosimetry; electron beams; microdensitometry; spectrophotometry; thin films.

It is possible to convert a conventional spectrophotometer into a versatile scanning spectrophotometer, without great difficulty or expense. The improved instrument can be tailored to perform many electro-optical tasks by the appropriate arrangement of modular components. In this work, basic optical components (light sources, monochromator, and sample chamber) of a conventional spectrophotometer were used on an optical bench. Specially designed accessories could be added to these components in order to measure at given wavelengths (from 200 to 800 nm) spatial variation (down to less than 10  $\mu\text{m}$ ) of optical transmission or reflection quantities in thin-film dosimeters, over a wide dynamic range. For high-speed data acquisition, analogue-to-digital conversion could be programmed to give tabular or graphical absorbed dose readings from calibrated film as a function of optical or spatial variables.

**12946.** Beatty, R. W., **Efficiencies of microwave 2-ports from reflection coefficient measurements**, *IEEE Trans. Microwave Theory Tech.* **MTT-20**, No. 5, 343-344 (May 1972).

**Key words:** Efficiency of two-port; measurement of 2-port efficiency; microwave measurements.

It is well-known that one can determine the efficiency of a microwave 2-port by measuring the reflection coefficient  $\Gamma_1$  at the input port when the output port is terminated by a sliding short circuit. The locus of  $\Gamma_1$  is a circle whose radius equals the efficiency  $\eta_{2m}$  for energy entering port 2 when port 1 is terminated in a nonreflecting load. Similarly  $\eta_{1m}$  is the radius of the  $\Gamma_2$  circle when port 1 is terminated in a sliding short circuit.

This note describes a procedure for obtaining, from the same measured data, new reflection coefficients  $\Gamma_{1N}$  and  $\Gamma_{2N}$ , whose circular loci have radii  $R_{1N}$  and  $R_{2N}$  which give the efficiencies of the 2-port when connected to an arbitrary load of reflection coefficient  $\Gamma_L$ .

Thus the  $\Gamma_1$  or  $\Gamma_2$  data may be used to obtain the efficiency of the 2-port when terminated in any arbitrary load. The method is potentially more accurate than the 3-point method since errors can be reduced by drawing a circle through many measured points.

**12947.** Arthur, M. G., **A precision HF-noise power measurement system**, *ISA Trans.* **10**, No. 3, 264-268 (1971).

**Key words:** Measurement system; noise comparator; noise measurement; noise standards.

This paper describes a precision HF noise power measurement system used at the National Bureau of Standards. It includes reference standard noise generators operating at approximately 77 and 373 K and an instrument for comparing the noise power of a noise source against the reference standards. The comparison instrument is a sum-and-difference correlation radiometer. Both the standards and the comparison instrument operate at 3, 30, and 60 MHz, and can be used with noise sources having source impedances of 50 ohms, unbalanced. Measurement uncertainty is typically less than 1% for sources with noise temperatures from 75 to 30,000 K.

**12948.** Fong, J. T., Simmons, J. A., **A non-equilibrium thermodynamic theory of simple materials based on a single-integral entropic functional**, (Proc. Int. Symp. on Foundations of Plasticity, Warsaw, Poland, Aug. 1972), *Arch. Mech. Stos.* **24**, No. 3, 363-372 (1972).

**Key words:** Anisotropy; continuum mechanics; entaxy; entropy; irreversibility; non-equilibrium state; nonlinear theory; plasticity; thermodynamics; viscoelasticity; yielding.

Based on the notion of a single-integral entropic functional as first introduced by Bernstein, Kearsley, and Zapas for a class of simple fluids in 1964, we present a non-equilibrium, irreversible thermodynamic theory of simple materials with fading memory within the general framework of Coleman's thermodynamic theory. Our theory is then modified, in a heuristic approach, to include "plasticity" by identifying the single-integral entropic functional with Bridgman's notion of "generalized entropy" for plastic deformations.

**12949.** Karp, S. S., Matteson, T. T., Maltese, M. D., **A search and rescue simulation model (SARSIM)**, *Proc. Tokyo 1971 AICA Symp. on Simulation of Complex Systems, Tokyo, Japan, Sept. 3-7, 1971*, pp. 1-4/1-1-4/8 (The Society of Analog Technique of Japan, Tokyo, Japan, Sept. 1971).

**Key words:** Manning levels; modeling; multiserver queuing system; resource locations; resource utilization; response system; simulation.



The United States National Bureau of Standards and the United States Coast Guard, in a joint endeavor, have designed and developed an effective simulation model of the Coast Guard's complex Search and Rescue system.

The Search and Rescue Simulation (SARSIM) simulates the operational selection of the preferred SAR resource(s) to respond to each distress client; clients' needs for Coast Guard assistance vary widely, both in type and amount. SARSIM is a discrete event digital simulation which is modularized to allow the user to prepare any demand scenario (with overall or selective growth factors) in the Preprocessor; to exercise that demand in the Operational Simulator, controlling such inputs as the mix of resources and the organizational operating structure (e.g., decentralization of facilities); to examine the summary results of the exercise through the automatic preparation of specified output statistics; and to employ the Postprocessor to retrieve additional information.

This paper describes the SARSIM model, including: some of its more interesting and flexible algorithms, some validation data and representative results of simulation exercises.

**12950.** Geltman, S., **Applications of pseudo-state expansions**, (Proc. VII Int. Conf. on the Physics of Electronic and Atomic Collisions, Amsterdam, July 26, 1971), Chapter in *Physics of Electronic and Atomic Collisions*, T. R. Gover and F. J. de Heer, eds. pp. 216-231 (North-Holland Publ. Co., Amsterdam, The Netherlands, 1972).

**Key words:** Close coupling; electron-atom scattering; polarizabilities; pseudo-states; Sturmians.

The various types of pseudo-state expansions which have been applied to the scattering of a charged particle by atoms are discussed. Of the applications so far made, greater success has been achieved in the case of low energy electron-hydrogen scattering than for high-energy proton-hydrogen scattering.

**12951.** Coyne, J. J., Meshkov, S., **High-energy total cross sections and symmetry relations**, *Phys. Rev. D* **6**, No. 1, 399-402 (July 1, 1972).

**Key words:** Barger-Rubin; Johnson-Treiman; SU(3), SU(6); symmetry; total cross sections.

Recent Serpukhov measurements of meson-baryon total cross sections allow comparisons with the Johnson-Treiman and Barger-Rubin relations. For 25-55-GeV/c incident meson momenta, the Johnson-Treiman relation,  $1/2\Delta(Kp) = \Delta(\pi p)$ , is well satisfied. The less restrictive Barger-Rubin relation holds for most of the Serpukhov points. Linear extrapolation of Serpukhov fits for  $\Delta(Kp)$  and  $\Delta(\pi p)$  to high momenta leads to the prediction of large violations of the Johnson-Treiman relations.

**12952.** Hockey, B. J., **Observations by transmission electron microscopy on the subsurface damage produced in aluminum oxide by mechanical polishing and grinding**, (Proc. British Ceramic Society Meeting, Textural Studies of Ceramics, London, England, Dec. 16-17, 1970), Paper No. 6 in *Textural Studies of Ceramics, Proceedings No. 20*, pp. 95-115 (British Ceramic Society, Shelton, Stoke-on-Trent, Great Britain, June 1972).

**Key words:** Aluminum oxide; dislocations; mechanical polishing and grinding; microtwins; transmission electron microscopy.

Transmission electron microscopy was used to examine the near-surface regions of  $Al_2O_3$  crystals which were: (1) polished with 0.25  $\mu m$  diamond, (2) polished with 0.3  $\mu m$  alumina powder, or (3) ground with a diamond-impregnated wheel.

Near-surface regions of diamond-polished polycrystalline and (0001) single-crystal sections contained a relatively uniform high

density of dislocations generally in the form of half-loops and closely associated with surface scratches. Similar subsurface damage, but to a lesser extent, was found in alumina-polished polycrystalline specimens. In both cases, depth of subsurface damage was estimated to be 1-2  $\mu m$ .

Observations on diamond-ground polycrystalline specimens at a depth of 2-4  $\mu m$  below the original surfaces (necessitated by the residual stresses and irregular topography) revealed penetrating arrays of dislocations and/or microtwins (basal and rhombohedral), depending on the orientation of the grain. Large numbers of basal twins, in particular, were found in diamond-ground (0112) specimens, while a (0001) section contained only non-basal dislocations. Maximum depth of damage produced by grinding was estimated to be  $\approx 20 \mu m$ .

The effect of briefly (1-4 hrs) annealing diamond-polished specimens at temperatures between 700 and 1500  $^{\circ}C$  was also investigated. Dislocation activity (and stress relief) was apparent after annealing at 900  $^{\circ}C$  and led to the development of large dislocation networks at 1200  $^{\circ}C$ . Annealing at 1500  $^{\circ}C$ , however, resulted in thermal etching and the elimination of nearly all subsurface damage.

**12953.** Hellwig, H., Bell, H. E., Kartaschoff, P., Bergquist, J. C., **Frequency stability of methane-stabilized He-Ne lasers**, *J. Appl. Phys.* **43**, No. 2, 450-452 (Feb. 1972).

**Key words:** Frequency stability; He-Ne laser; laser stabilization; length standard; methane frequency standard; saturated absorption; time standard.

Free-running laser stabilities of  $1.5 \times 10^{-11}$  for the millisecond region and methane-locked stabilities of  $10^{-13}$  for 10-sec averaging time are achieved with a minimum of shock and vibration isolation in an ordinary laboratory environment. Superior stability performance is obtained with dc excitation as compared to rf excitation. The experimental setup is described in some detail.

**12954.** Kamper, R. A., Simmonds, M. B., **Broadband superconducting quantum magnetometer**, *Appl. Phys. Lett.* **20**, No. 8, 270-272 (Apr. 15, 1972).

**Key words:** Magnetometer; microwaves; quantum interference; superconductivity.

We describe the design, operation, and performance of a superconducting quantum interference device (SQUID) which operates at a frequency of 9 GHz. It is sensitive to variations of magnetic field in a frequency band from 0 to 1 GHz.

**12955.** Grimes, D. N., **Optical autocorrelator with special application to MTF measurement**, *Appl. Opt.* **11**, No. 4, 914-918 (Apr. 1972).

**Key words:** Autocorrelation; interferometry; lens testing; modulation transfer function; optics; physical optics; Sagnac interferometer.

An optical autocorrelator is described which is based on a modified Sagnac two-mirror interferometer that operates in the zero-fringe mode. The real-time radiant flux output is the square of the autocorrelation of the aperture function. In a particular application, when the aperture function is the pupil function of a lens under test, the autocorrelator output is the MTF of the lens. The system is not limited in focal length; aperture size is limited only by the sizes of the beam splitters and mirrors. Experimental results are given with comparison data for both infinite-conjugate MTF and the autocorrelation of an annular aperture. Methods of adapting the system for measurement of the phase of the transfer function and for finite conjugate testing are also described.

**12956.** Hils, D., McCusker, M. V., Kleinpoppen, H., Smith, S. J., **Differential and direct differential elastic scattering cross sec-**



tions for electrons and potassium atoms, *Phys. Rev. Lett.* **29**, No. 7, 398-401 (Aug. 14, 1972).

Key words: Cross sections; elastic scattering; spin polarization.

In a modulated crossed-beam experiment we have elastically scattered unpolarized electrons of 3.3 eV energy from spin-polarized K atoms. A measurement of the polarization of the scattered electron yields  $|f(\theta)|^2/\sigma(\theta)$ . Our measured values of  $|f|^2/\sigma(\theta)$  show a significant angular shift relative to the theoretical curve in forward-angle scattering ( $\theta = 20 - 40^\circ$ ). This shift is not apparent in measurements of the differential scattering cross section  $\sigma(\theta)$  over the same angular range, which, however, do show a significant angular shift in the range  $\theta = 50 - 120^\circ$ .

**12957.** Kartaschoff, P., Barnes, J. A., **Standard time and frequency generation**, *Proc. IEEE* **60**, No. 5, 493-501 (May 1972).

Key words: Accuracy; basic standards; frequency; frequency metrology; stability; standards; time scales.

The basic properties of atomic primary frequency standards are reviewed. A continuously running frequency source combined with counting, storage, and display devices results in a clock. Time scales are obtained by setting clocks with respect to a convenient origin. The accuracy of a primary frequency standard is a combined theoretical and experimental assessment of the uncertainties of all known possible sources of bias from the idealized definition. Recommended standard measures for the stability are the spectral density of fractional frequency fluctuations (frequency domain) and the two-sample no-dead time Allan variance (time domain). The operation of atomic frequency standards is based on various methods of particle interrogation to observe the transitions, particle confinement to obtain sufficient interaction time, and particle preparation to obtain the desired energy level populations. Passive resonator and active oscillator (maser) modes of operation are discussed; the former has some fundamental advantages.

A review of the state of the art and current practice shows that cesium beam resonator standards have the best documented accuracy capability ( $5 \times 10^{-13}$ ) and, in their commercial versions, are presently the best available clocks.

There are three concepts related to time: time interval, date, and synchronization. In order to assign dates to events, time scales have to be established. The steadily growing need for a very precise and uniform time scale has resulted in a new internationally coordinated time scale, IAT.

Frequency metrology will have increasing impact on both length and voltage metrology in the near future.

**12958.** Wells, J. S., Evenson, K. M., Day, G. W., Halford, D., **Role of infrared frequency synthesis in metrology**, *Proc. IEEE* **60**, No. 5, 621-623 (May 1972).

Key words: Frequency metrology; frequency of lasers; infrared frequency synthesis; laser frequency stabilization; methane-stabilized He-Ne laser; speed of light.

Infrared frequency synthesis (IFS) techniques are briefly surveyed, and some important results are summarized. The recent measurement of the frequency of the methane-stabilized He-Ne laser is significant due to the accurate measurement of the methane wavelength and its fundamental role in metrology. The possibilities of an improved value for the speed of light and of additional applications for frequency measurements at various levels of accuracy are discussed.

**12959.** Allan, D. W., **Time transfer using near-synchronous reception of optical pulsar signals**, *Proc. IEEE* **60**, No. 5, 625-627 (May 1972).

Key words: Accurate time dissemination; optical pulsars; precision timing; simultaneous reception; synchronization; time transfer.

The concept of time transfer between two geographically separated locations by using nearly simultaneous reception times from a common transmission has been used very fruitfully, e.g., the TV line-10 time transfer system and Loran-C. Some germane aspects of the concept are discussed and use of a signal from the optical pulsar NP0532 as the common transmitter is considered.

Theoretical considerations suggest that time could be transferred using this mode to an accuracy of about  $2 \mu\text{s}$  and with global coverage. Some data were made available from Lawrence Radiation Laboratory giving the dates of pulsar events received at their observatory and also at the Harvard Observatory. A precision of about  $13 \mu\text{s}$  was inferred from the data analysis.

This optical pulsar time transfer system seems to be feasible and worthy of further consideration because of the high accuracy and precision (a few microseconds for both) potentially achievable. For this potential, the development costs appear to be favorably competitive.

**12960.** Halford, D., Hellwig, H., Wells, J. S., **Progress and feasibility for a unified standard for frequency, time, and length**, *Proc. IEEE* **60**, No. 5, 623-625 (May 1972).

Key words: Cesium beam frequency standard; dissemination systems; EMF standard; frequency and time metrology; frequency standards; infrared frequency synthesis; International System of Units; Josephson effect; length standards; methane frequency standard; speed of light; unified standard.

The recent successful extension of frequency synthesis upward in the infrared to the 88-THz frequency of the very stable methane frequency standard has implications for expanded uses of frequency/time metrology and hence of frequency/time dissemination systems. After further refinements of the infrared frequency synthesis techniques, metrologists will have the opportunity to define a value for the speed of light and to use a particular frequency standard—the most accurate one—as a unified standard for frequency, time, and length.

**12961.** Penn, R. W., **Volume changes accompanying the extension of rubber**, *Trans. Soc. Rheol.* **14**, No. 4, 509-517 (1970).

Key words: Compressibility; natural rubber; strain energy; volume-extension.

The volume changes accompanying extension of peroxide vulcanizates of natural gum rubber were measured using a dilatometer technique. Measurements of the force-extension behavior and compressibilities were made on the same samples for the range of extension and volume change covered in the volume experiments. A constant compressibility was found; however, the volume changes accompanying extension were not proportional to the isotropic part of the stress. Thus, the strain energy cannot be separated into a sum of two parts, one due to the shear and one due to the dilatation.

**12962.** Artru, M-C., Kaufman, V., **Analysis of the spectrum of triply-ionized magnesium (Mg IV)**, *J. Opt. Soc. Amer.* **62**, No. 8, 949-957 (Aug. 1972).

Key words: Magnesium; source; spectra; ultraviolet; wavelengths.

A study of Mg IV between 80 and  $2100 \text{ \AA}$  has led to the classification of 243 lines. A total of 23 odd and 64 even levels have been identified as belonging to the  $2s^2 2p^5$ ,  $2s 2p^6$ ,  $2s 2p^5 3s$ ,  $2s^2 2p^4 4p$ ,  $2s^2 2p^4 ns$ , and  $2s^2 2p^4 nd$  ( $n=3, 4, 5$ ) configurations. Matrix diagonalizations and least-squares fits to the observed



levels lead to well-defined radial integrals and verify the level assignments. On the basis of comparisons in the F 1 isoelectronic sequence, designation changes are suggested for some  $2p^4(3P)3d$  levels of Na III, Al V, Si VI, P VII, and S VIII. New levels are given for Na III and Al V, and some previously listed levels in Na III and S VIII are rejected as unreal. An ionization energy of  $880\,800\text{ cm}^{-1}$  is given for Mg IV.

**12963.** Ivey, D. L., Keese, C. J., Neill, A. H., Jr., Brenner, C., **Interaction of vehicle and road surface**, *Highw. Res. Rec., Anti-Skid Program Management and Related Papers, 22 Reports*, No. 376, 40-53 (1971).

Key words: Brakes; coefficient of friction; skid testers; tire construction; traction.

This paper presents various factors which influence friction forces in the interaction between the vehicle and the road surface. Emphasis has been directed toward interpretation of slip curves and how they relate to total vehicle handling.

The effects of braking systems, locked wheels, antilock brakes, and suspensions are related to actual vehicle performance data. Likewise, variations in construction and tread depth are evaluated on both wet and dry surfaces.

**12964.** Powell, C. J., **Internal x-ray photoemission in aluminum: Excitation of electrons from the valence bands**, *Solid State Commun.* **10**, No. 12, 1161-1164 (June 15, 1972).

Key words: Aluminum; electronic density of states; photoelectron energy distribution; x-ray photoemission.

Measurements are reported of Al valence-electron excitation by  $K\alpha_{1,2}$  x-rays internally generated in evaporated specimens by electron bombardment. The x-ray photoelectron energy distribution is consistent with the u.v. distributions of Huen and Wooten. Weak structures are found in the energy distribution at positions corresponding to those in the calculated density of states.

**12965.** McDaniel, C. L., **Phase relations in the CaO-Pt system in air**, *J. Amer. Ceram. Soc. Discussions and Notes* **55**, No. 8, 426-427 (Aug. 1972).

Key words: CaO-Pt system; CaO:PtO<sub>2</sub> compounds; dissociation; equilibrium; phase relations.

The equilibrium phase relations for the CaO-Pt system were determined in an air environment. The system contains two compounds  $4\text{CaO} \cdot \text{PtO}_2$  and  $\text{CaO} \cdot \text{PtO}_2$  which dissociate to an oxide phase, Pt metal, and oxygen at 1035 and 905 °C, respectively. An indexed x-ray diffraction powder pattern is given for the  $4\text{CaO} \cdot \text{PtO}_2$  compound.

**12966.** Franklin, A. D., **Statistical thermodynamics of point defects in crystals**, Chapter 1 in *Point Defects in Solids*, J. Crawford and L. Slifken, eds., 1, 1-101 (Plenum Press, Inc., New York, N.Y., 1972).

Key words: Formation enthalpy; formation entropy; formation free energy; formation volume; ionic solids; metals; noble gas solids; point defects; semiconductors; statistical thermodynamics.

A review is given of the statistical and thermodynamic theory of point defects in dilute solution in noble gas solids, metals, semiconductors, and ionic solids. Experimental methods for determining the free energies, enthalpies, entropies, and volumes of formation of single and complexed point defects are reviewed, and a survey is given of the available values at the present time.

**12967.** Sullivan, D. B., **Low temperature voltage divider and null detector**, *Rev. Sci. Instrum.* **43**, No. 3, 499-505 (Mar. 1972).

Key words: Null detector; superconductivity; voltage divider.

This paper describes a low temperature voltage divider and null detector which are designed to accurately bring the low level voltage of the Josephson steps to the 1 V level. The divider uses the series-parallel interchange of resistors. Preliminary tests indicate that the resistors are stable to within one part in  $10^7$  and that the ratio is accurate to within one part in  $10^6$ . The null detector utilizes a superconducting quantum interference magnetometer and is limited only by the Johnson noise in the cooled resistors.

**12968.** Meijer, P. H. E., **Specific heat and susceptibility in chromium methylammonium alum above the critical temperature**, *Phys. Rev. B* **6**, No. 1, 214-222 (July 1, 1972).

Key words: Chromium methylammonium alum; crystal field; high-temperature expansion; specific heat; susceptibility.

The specific heat and susceptibility of chromium methylammonium alum is calculated above the critical temperature. The method is based on a high-temperature expansion of the partition function in the presence of a crystal field, using a Laplace transform. The results are worked out in first (for the susceptibility) and second (for the specific heat) order in the coupling Hamiltonian. The summation over the four different sublattices is worked out for the two different crystallographic phases which seem to occur above and below 170 K. The lack of rotation symmetry of the crystal field in its local reference system, which was found by paramagnetic resonance, is taken into account. The result for the susceptibility is given explicitly in Eq. (4.18a) as a function of a reduced temperature.

**12969.** Krauss, M., Neumann, D., **Energy curves of  $\text{CO}_2^-$** , *Chem. Phys. Lett.* **14**, No. 1, 26-28 (May 1, 1972).

Key words:  $\text{CO}_2^-$ ; electron scatter; energy curve; excitation energy; metastable; quantum chemistry.

*Ab initio* energy curves of the  $^2A_1$  and  $^2B_1$  states of  $\text{CO}_2^-$  are reported as a function of the bending angle. The  $^2A_1$  curve is found to be bound relative to the neutral curve at angles greater than  $130^\circ$  from the linear geometry. Both the  $^2A_1$  and  $^2B_1$  states are found to be valence in character for the geometries considered and the excitation energy for  $^2A_1 \rightarrow ^2B_1$  is calculated to be 3.2 eV in the neighborhood of the  $\text{Co}_2^-$  equilibrium geometry while the experimental value for the maximum in the lowest absorption curve is almost 3.5 eV.

From the bending energy curve it is deduced that gaseous  $\text{CO}_2^-$  in its ground vibrational level can have a relatively long life since the ion energy in the neighborhood of the ion equilibrium geometry is about 1 eV below the neutral molecule energy for that geometry.

**12970.** Linzer, M., Brown, R. L., **Line parameters of absorption and dispersion Lorentzian curves under conditions of combined modulation and saturation distortion**, *J. Magn. Resonance* **7**, 335-358 (1972).

Key words: Line shapes; Lorentzian lines; magnetic resonance.

Analytical and computer solutions for the parameters of the first Fourier coefficients of Lorentzian lines subject to simultaneous modulation and saturation distortion are presented. Both absorption and dispersion shape functions are examined. The system is assumed to be described by the saturation theory of either Bloembergen, Purcell, and Pound (BPP), or Redfield. In the BPP case, results are given for the modulation frequency,  $\omega_m$ , being much greater or less than  $1/T_1$ , while in the Redfield case, only  $\omega_m \ll 1/T_1$  is considered. In all cases, it is assumed that  $\omega_m/2\pi$  is much less than the inverse line width of the pure ab-

sorption curve and that the line is traversed during a time which is slow compared to  $T_1$  and  $2\pi/\omega_m$ .

Various methods are outlined for determining the true line width, line intensity, saturation parameter, and modulation amplitude from measurements on the distorted line shapes under conditions of optimum sensitivity. Tests for verifying the character of the Lorentzian line shape are also suggested.

**12971.** Brown, R. L., Use of fiber optics in the study of chemiluminescent reactions, *Rev. Sci. Instrum.* **43**, No. 5, 756-758 (May 1972).

Key words: Chemiluminescent reactions; fiber optics; photochemistry.

The use of stationary light pipes and a stationary detector to measure light decay along a tube in a steady state flow system is described. This method exhibits a number of advantages over that of moving the detector. A means of calibrating the transmission of the light pipes *in situ* by using the properties of the yellow nitrogen afterglow is discussed. The high degree of spatial resolution achievable by this technique should make it especially suitable for studies of small flames and discharges.

**12972.** Mangum, B. W., Utton, D. B., NMR of  $^{14}\text{N}$  in cerous magnesium nitrate hydrate, *Physica* **60**, No. 1, 63-72 (1972).

Key words: CMN; ideal paramagnet; NMR; NQR.

We have measured the nuclear magnetic resonance of  $^{14}\text{N}$  in cerous magnesium nitrate hydrate,  $\text{Ce}_3\text{Mg}_3(\text{NO}_3)_{12} \cdot 24\text{H}_2\text{O}$ , at 1 K in a magnetic field of 18.335 kG. The dipolar field at the nitrogen nucleus due to the  $\text{Ce}^{3+}$  ions is appreciable at that temperature and field and produces phase shifts in the angular dependence of the spectra. This complicates the interpretation of the data and prevents one from using the customary techniques. From the measurements we have derived values for the quadrupolar coupling constant ( $A = 0.160 \pm 0.005$  MHz), the asymmetry parameter ( $\eta = 0.50 \pm 0.05$ ) and the directions of the electric-field gradient axes. The spectra show clearly that for the nitrate groups there is no center of inversion at the cerium ions.

**12973.** Allan, D. W., Blair, B. E., Davis, D. D., Machlan, H. E., Precision and accuracy of remote synchronization via network television broadcasts, Loran-C, and portable clocks, *Metrologia* **8**, No. 2, 64-72 (Apr. 1972).

Key words: Allan variance; cesium beam standards; frequency stability; frequency standards; Loran-C; portable clocks; time dispersion; time synchronization; TV timing.

A comparison among three precise timing centers in the United States has been conducted for more than 1 year using three different synchronization methods. The timing centers involved were the United States Naval Observatory (USNO) in Washington, D.C., Newark Air Force Station (NAFS) in Newark, Ohio, and the National Bureau of Standards (NBS) in Boulder, Colorado. The three methods were cesium beam portable clocks; Loran-C transmissions from Cape Fear, North Carolina, and Dana, Indiana; and ABC, CBS, and NBC network television broadcasts commonly received by the three timing centers.

Cesium beam portable clocks have the capability of accurately and precisely synchronizing remote clocks to within  $0.1 \mu\text{s}$ . The Loran-C data involved a 3500 km (2180 miles) ground wave path—the longest Loran-C ground wave path that has been studied with the precision and accuracy reported herein. The long-term precision achieved was about  $1 \mu\text{s}$  over 1 year. The accuracy is limited on occasion by inability to resolve the  $10 \mu\text{s}$  ambiguity of the 100-kHz pulse train. The precision capability of maintaining remote clock synchronization within the majority of

the continental United States using network television broadcasts was inferred to be about  $5 \text{ ns} \cdot \tau^{1/3} \text{s}^{-1/3}$  over the range of  $\tau$  from 86400 s (1 day) to about  $10^7$  s (324 days) but with definite accuracy limitations caused by such factors as occasional network re-routing of the television signals. Some estimates of the long-term frequency stabilities among the references used at the three timing centers were measured or inferred.

**12974.** Clark, A. F., Deason, V. A., Powell, R. L., Characterization of high purity metals by the eddy current decay method, *Cryogenics* **12**, No. 1, 35-39 (Feb. 1972).

Key words: Contaminants; cryogenics; eddy currents; eddy current tests; electrical resistivity; nondestructive tests; purity; scattering.

In recent years, the residual resistivity ratio has been widely used as a sensitive indicator of chemical purity in high purity metals. The conventional four terminal measurement of resistivity becomes difficult either with large or irregular specimens or with increasing purity and decreasing temperature. This paper describes an alternative technique, called the eddy current decay method, which greatly reduces the above difficulties. The eddy current measurements do not require any attachment of leads and, in fact, the measurement process is totally non-destructive to the specimen. The eddy current apparatus is described, and some typical applications are presented.

**12975.** Sparks, L. L., Powell, R. L., Methods for assessing homogeneity and interchangeability of thermocouple wires, *Cryogenics* **12**, No. 1, 40-43 (Feb. 1972).

Key words: Cryogenics; dipping; evaluation; heterogeneity; liquid helium; liquid nitrogen; low temperature; Seebeck effect; temperature measurement; thermoelectric properties.

Chemical and physical imperfections and inhomogeneities in thermocouple wire cause spurious voltages whenever these imperfections are subjected to temperature gradients. Thermocouple wires from different spools (or even from widely separated lengths on the same spool) usually exhibit significant differences in their thermoelectric properties. For accurate thermometry it is important to know the range of spurious voltages to be expected from a specific material. Simple laboratory methods are described for determining the effects of short-range inhomogeneities or long-range variations. Examples of results from tests are discussed in order to point out both the usefulness and the limitations of the methods.

**12976.** Jackson, A. D., Maximon, L. C., Integrals of products of Bessel functions, *SIAM J. Math. Anal.* **3**, No. 3, 446-460 (Aug. 1972).

Key words: Angular momentum algebra; Bessel functions; integrals of Bessel functions; invariant triple products; spherical Bessel functions; spherical harmonics.

Simple expressions for a variety of integrals involving the product of three cylindrical or three spherical Bessel functions are obtained in terms of the angular functions arising in the decomposition of a plane wave in two or three dimensions.

**12977.** McKinney, J. E., Penn, R. W., Composite dilatometer for measuring density of liquids and solids, *Rev. Sci. Instrum.* **43**, No. 8, 1211-1213 (Aug. 1972).

Key words: Compressibility; density; dilatometer; pressure; specific volume; temperature; thermal expansion.

A composite dilatometer for measuring densities of liquids and solids over wide ranges of temperature and pressure is described. The dilatometer has a glass capillary and a mechanically remova-



ble seal at the base to facilitate loading. The seal is leakproof, and constant volume is maintained with successive loadings.

12978. Kelly, G. E., Sengers, J. V., **Kinetic theory of droplet growth in nucleation**, *J. Chem. Phys.* 57, No. 4, 1441-1458 (Aug. 15, 1972).

**Key words:** Droplet growth; inverse Knudsen number expansion; kinetic theory; nearly-free molecular regime; nucleation.

A kinetic theory is presented for the mass flux to a liquid droplet surrounded by its pure vapor. When the mass flux  $\Gamma$  is expanded in terms of a parameter  $\alpha$  which is the ratio of the droplet size to the mean free path (inverse Knudsen number), one obtains a series of the form  $\Gamma = \Gamma^{(0)} + \Gamma^{(1)}\alpha + \Gamma^{(2)}\alpha^2 \ln\alpha + \dots$ . The coefficients of the first three terms of this expansion are derived by solving the Boltzmann equation using a modified Knudsen number iteration procedure. It is shown that the coefficients are determined by integrals associated with sequences of successive collisions among a number of vapor molecules and the droplet. These collision integrals bear a close similarity to the collision integrals derived earlier from the *generalized* Boltzmann equation for the density dependence of the transport properties of gases.

12979. Waxman, M., Hastings, J. R., **Proposed experiment to determine the effect of pressure on the emf of thermocouples**, *J. Appl. Phys.* 43, No. 6, 2629-2632 (June 1972).

**Key words:** emf, thermocouple, effect of pressure on; hot-junction temperature, nonlinear evaluation of; hot-junction temperature, pressurized furnace; indirect temperature measurements; nonlinear data analysis, pressurized emf of thermocouples; pressure, effect on emf of thermocouples; simulated experiment, pressurized emf of thermocouples; temperature, measurement at high pressure; thermocouples, effect of pressure on emf of.

A new experimental procedure to determine the effect of pressure on the emf-vs-temperature behavior of thermocouples has been conceived and tested with simulated data on a computer. An important advantage of this procedure is that the temperature of the hot junction can be accurately evaluated without the necessity of measuring it directly. Instead, the emf of the pressurized thermocouple is expressed parametrically as an appropriate function of several variables: (i) a measurable property related to the hot-junction temperature, such as the electric power to the pressurized furnace; (ii) the cold-junction temperature; and (iii) a reference temperature, such as 100 °C, at which the pressure effect is known. By variation of the experimental conditions, a set of overdetermined equations is obtained from which the parameters can be evaluated, and thus the emf-vs-temperature relationship of the pressurized thermocouple can be determined. Our experience with simulated data indicates that for the temperature range from 100 to 1200 °C and for pressures to about 7 GN/m<sup>2</sup> (70 kbar), the procedure should not introduce a temperature error greater than the error associated with the measurements of the emf, power, and cold-junction temperature.

12980. MacDonald, R. A., **Cauchy relations for second- and third-order elastic constants**, *Phys. Rev. B* 5, No. 10, 4139-4143 (May 15, 1972).

**Key words:** Cauchy relations; central force interaction; cubic crystals; second- and third-order elastic constants; stress-free equilibrium; third-neighbor model.

The results of an earlier paper on the relation between elastic constants and second- and third-order force constants in face-centered-cubic and body-centered-cubic lattices appeared to conflict with the Cauchy relations  $C_{12} = C_{44}$ ,  $C_{112} = C_{166}$ ,  $C_{123} =$

$C_{456} = C_{144}$  obtained by Cousins. We show here that no conflict exists when we ensure that the lattice is in stress-free equilibrium, a necessary condition for Cauchy relations to hold. However, for the case of nearest- and next-nearest-neighbor central-force interactions previously considered, we obtain only special cases of these Cauchy relations. We extend our earlier work to include further neighbors and find that the Cauchy relations are obtained when third neighbors contribute to the elastic constants.

12981. Cassidy, E. C., **Pulsed laser Kerr system polarimeter for electro-optical fringe pattern measurement of transient electrical parameters**, *Rev. Sci. Instrum.* 43, No. 6, 886-893 (June 1972).

**Key words:** Electric fields; electrical measurements; electro-optics; high-speed photography; high-speed techniques; high-voltage techniques; Kerr effect; laser application; optical techniques; pulse techniques.

Novel electro-optical fringe pattern methods are developed for measurement of transient high voltages and electric fields. Several techniques employing the Kerr effect, a pulsed laser source, and high-speed photographic recording equipment are described. Typical fringe pattern results are compared with conventional resistive divider measurements.

12982. Hellwig, H., Bell, H. E., **Experimental results with atomic hydrogen storage beam systems**, *Proc. 26th Annual Symp. on Frequency Control, Atlantic City, N.J., June 6-8, 1972*, pp. 242-247 (Electronic Industries Association, Washington, D.C., June 6-8, 1972).

**Key words:** Atomic hydrogen beam; atomic hydrogen generation; dispersion; frequency stability; frequency standard; hydrogen atom detection; hydrogen flux calibration; hydrogen maser; relaxation measurements; spin exchange.

Two atomic hydrogen storage beam devices are described, one based on the detection of hydrogen atoms, the other on the detection of changes in the microwave signal due to the hydrogen resonance. Electron bombardment ionization is used for the detection of atomic hydrogen. Efficiencies of up to  $10^{-3}$  are measured using a method which is based on the study of pulse decay at maser oscillation threshold. Quantitative measurements of the atomic hydrogen beam intensity as a function of source pressure and RF discharge power are given. The overall efficiency of the atomic hydrogen detection in the hydrogen storage beam device is estimated at  $10^{-7}$ . Ways to increase the efficiency are indicated.

A frequency standard is described in which a quartz crystal oscillator is locked to the hydrogen hyperfine transition using the dispersion of this resonance. The hydrogen storage beam apparatus closely resembles a hydrogen maser with a low-Q cavity below oscillation threshold. Cavity pulling can be reduced to a point where environmental temperature fluctuations limit the stability mainly via the second-order Doppler effect. Locking to the dispersion feature of the resonance eliminates the need for frequency modulation in order to find line-center. The stability of the frequency standard was measured against crystal oscillators and cesium beam frequency standards; stabilities of  $4 \times 10^{-13}$  were recorded for sampling times of 30 seconds and of 3 hours.

12983. Mangum, B. W., Thornton, D. D., **Magnetic phase diagrams of GdVO<sub>4</sub> and GdAsO<sub>4</sub>**, (Proc. 17th AIP Conf. on Magnetism and Magnetic Materials, Chicago, Ill., Nov. 16-19, 1971), Chapter in *Magnetism and Magnetic Materials*, C. D. Graham, Jr., and J. J. Rhyne, eds., No. 5, 311-315 (1972).

**Key words:** GdAsO<sub>4</sub>; GdVO<sub>4</sub>; Heisenberg antiferromagnets; low temperatures; magnetizations.



GdAsO<sub>4</sub> and GdVO<sub>4</sub> are Heisenberg antiferromagnets with relatively large anisotropy fields, about half of which are dipolar in origin. The ratios of the anisotropy to the exchange fields for the salts, based on the molecular field theory and using the published values of the interaction constants, indicate that both salts should have spin-flop phases. We have measured the magnetization and its derivative of GdVO<sub>4</sub> and GdAsO<sub>4</sub> as a function of applied magnetic field for various temperatures below  $T_N$  and derived their magnetic phase diagrams. GdVO<sub>4</sub> ( $T_N = 2.50$  K) is a textbook type example of a system having a spin-flop phase with  $T_3 = 1.37$  K. The critical field for the transition from the antiferromagnetic to the spin-flop phase is 10.5 kG and that for the transition from the spin-flop to the ferromagnetic (or saturated paramagnetic) phase is 21.8 kG. GdAsO<sub>4</sub> ( $T_N = 1.26$  K) does not have a simple spin-flop phase but undergoes transitions to two intermediate phases before undergoing a transition to the ferromagnetic (or saturated paramagnetic) phase. The critical point for GdAsO<sub>4</sub> is  $T_c = 0.47$  K and the critical fields are:  $B_{c1} = 6.1$  kG,  $B_{c2} = 6.4$  kG, and  $B_{c3} \approx 9$  kG.

12984. Rubin, L. G., Powell, R. L., Anderson, A. C., Conference Report—The Fifth Symposium on temperature, *Cryogenics* 11, No. 6, 489-493 (Dec. 1971).

Key words: Temperature scales; thermocouples; thermometry.

The review briefly describes the talks on thermocouples and temperature scales. The article mentions the authors, their affiliations, and brief synopses of the more significant talks.

12985. Weiss, A. W., Calculations of the  $2s_{ns} \ ^1S$  and  $2p3p \ ^3,1P$  levels of Be I, *Phys. Rev. A* 6, No. 4, 1261-1266 (Oct. 1972).

Key words: Atomic spectra; lifetimes; oscillator strengths; wavelengths.

Large scale configuration-interaction calculations are carried out on the  $2s_{ns} \ ^1S$  series of Be I in an attempt to account for the anomalous behavior of the measured  $f$  values for the 3455-Å line, which had been identified as the  $2s2p \ ^1P - 2p^2 \ ^1S$  transition. The calculations indicate that the series is very nearly purely Rydberg in character and that  $2p^2 \ ^1S$  is not embedded in the series between  $6s$  and  $7s$ , as had been previously assigned. Additional variational calculations on the  $2snp$  and  $2p3p$  levels indicate that a reidentification of the 3455-Å line with the  $2s3p \ ^1P - 2p3p \ ^1P$  transition is consistent with both lifetime and wavelength measurements. These calculations also predict lines at 2148 and 4528 Å, which have recently been found in beam-foil spectra.

12986. Allan, D. W., Machlan, H. E., Marshall, J., Time transfer using nearly simultaneous reception times of a common transmission, *Proc. 26th Annual Symp. on Frequency Control, Atlantic City, N. J., June 6-8, 1972*, pp. 309-316 (Electronic Industries Association, Washington, D.C., June 6-8, 1972).

Key words: Atomic clock; frequency calibration; frequency stability; optical pulsars; remote clock comparisons; simultaneous reception; time dissemination; time stability; time synchronization; time transfer; TV color subcarrier; 60-Hz power line.

The concept of time transfer between two geographically separated locations by using nearly simultaneous reception times of a common transmission has been used very fruitfully, e.g., the TV line-10 time transfer system and Loran-C. This paper discusses some germane aspects of the concept and then considers using as some common transmissions a 30-Hz pulsed signal from the optical pulsar NP0532, the 60-Hz power-line signal, and the 3.58-MHz television color subcarrier signal.

The theoretical accuracy of each of these methods is discussed along with its coverage and the system feasibility. The day-to-day stability of the differential path delay of each of the above methods was measured or inferred to be  $\sim 13 \mu s$ ,  $\sim 1$  ms, and  $\sim 20$  ns respectively.

12987. Smith, J. C., Kermish, G. A., Fenstermaker, C. A., Separation of filler particles from the matrix in a particulate-loaded composite subjected to tensile stress, (Proc. ACS Symp. on Recent Advances in Adhesion, Washington, D.C., Sept. 13-15, 1971), *J. Adhes.* 4, No. 2, 109-122 (1972).

Key words: Adhesion; composite materials; epoxy polymer; silane coupling agents; stress-strain properties.

Simultaneous measurements of tensile stress, longitudinal strain, and transverse strain were obtained on particulate-filled composites. The matrix was a flexible epoxy polymer. Small glass spheres were used as filler in various volume ratios up to 0.35. The spheres were pretreated as follows: clean, coated with a parting agent, coated with either of two silane coupling agents. The volume-expansion behaviors of these four systems of composites showed differences attributed to matrix-filler separation and subsequent vacuole formation. Stress-strain behaviors were especially sensitive to this dewetting process. These two types of data, obtained simultaneously and considered together, thus provide valuable information about interface adhesion.

12988. Schooley, J. F., Soulen, R. J., Jr., Thermometric fixed points using superconductivity, *Advan. Cryog. Eng.* 17, 192-198 (1972).

Key words: Calibration techniques; cryogenic temperature scale; OSRM; pure elements; superconductivity; thermometric fixed points.

Superconductive transitions in lead, indium, aluminum, zinc, and cadmium samples have been found to be both narrow and reproducible, suggesting their use as calibrating fixed points on the cryogenic temperature scale. Devices based on these measurements have been constructed. These results and their use in cryogenic thermometry are discussed.

12989. Mangum, B. W., Utton, D. B., Low-temperature transitions in tetramethylammonium manganese chloride, *Phys. Rev. B* 6, No. 7, 2790-2795 (Oct. 1, 1972).

Key words: Cooperative transition; magnetic susceptibility; NMR; TMC.

We have measured the proton nuclear magnetic resonance of tetramethylammonium manganese chloride, a linear chain antiferromagnet, in the temperature region 0.4-300 K. In addition, its ac magnetic susceptibility was measured in applied fields of 0 to 22 kG in the temperature range 0.3-4.2 K. When measured along the crystallographic  $c$  axis, the zero-field susceptibility had an anomaly at 0.84 K. When the external field was applied perpendicularly to the  $c$  axis below 0.8 K, a critical field of 11.5 kG was observed in  $dM/dB$ . The proton NMR did not indicate any cooperative transition to a magnetically ordered state of the  $Mn^{2+}$  spins. It did indicate, however, a gradual diminution of fluctuations in the crystallographic  $ab$  plane until a nonrandom order had been established between chains below approximately 0.8 K. We find that the tetramethylammonium groups cease all rotations below 39 K. In the region of 40 to 50 K, the tetramethylammonium groups not only undergo some hindered rotations, but their orientation is different from the published room-temperature x-ray diffraction results. Above 50 K only a single narrow NMR line is observed and, consequently, no additional information on the crystal structure could be obtained.



**12990.** Colwell, J. H., Mangum, B. W., **The heat capacity of TmAsO<sub>4</sub> near its Jahn-Teller transition; evidence of a low-lying excited state**, *Solid State Commun.* **11**, 83-87 (1972).

**Key words:** Heat capacity; Jahn-Teller effect; molecular field approximation; Schottky anomaly; thulium arsenate; TmAsO<sub>4</sub>.

We have measured the heat capacity of TmAsO<sub>4</sub> between 2 and 12 K and have established that there is a singlet state at approximately 20 K (14 cm<sup>-1</sup>) above the ground state doublet. The heat capacity is accounted for on the basis of models which, in addition to the contribution from the low-lying singlet state, use the molecular field model to approximate the heat capacity arising from the Jahn-Teller splitting of the ground state doublet.

**12991.** Branscomb, L. M., **A metric America—and the paper industry**, *Tappi* **55**, No. 8, 1227-1230 (Aug. 1972).

**Key words:** Changeover; foreign trade; metric system; paper machines; planning; standards; United States; units of measures.

A study by the U.S. Department of Commerce clearly favors changeover to the metric system. There are two alternatives for the United States: to convert deliberately with a plan, or to go metric eventually without a plan. The change to the metric system will be costly and is not enthusiastically supported by the paper industry. Moreover, problems of adjustment will be great for the consumer in the market place. However, economic benefits of "going metric" may be achieved for a long time by making products conform to international standards developed by IEC and ISO. By conversion to the metric system, American industry could eliminate the necessity of keeping inventories of metric parts alongside customary parts. For the paper industry, conversion provides an opportunity to rationalize and simplify paper sizes. In addition, large economic benefits may be achieved through a rational, simplified series of package sizes. Thus, the paper industry will not be forced to scrap existing machinery; only those parts essential to producing products conforming to international standards need be changed.

**12992.** Tate, E. L., **NBS and the field service libraries of the Department of Commerce and the Interior Department**, *Proc. U.S. Department of Interior, Sixth Annual Library Workshop, Vancouver, Wash., Sept. 27-Oct. 1, 1971*, pp. 65-68 (U.S. Department of Interior, Office of Library Services, Washington, D.C., 1972).

**Key words:** National Bureau of Standards publication; National Standard Reference Data System.

Describes NBS services and publications of potential utility to the Department of the Interior and the Department of Commerce and their field service libraries.

**12993.** Pfrang, E. O., Yokel, F. Y., **Evaluation of innovative structural systems with respect to creep buckling**, *Proc. RILEM Int. Symp. on Experimental Analysis of Instability Problems on Reduced and Full-Scale Models, Buenos Aires, Argentina, Sept. 13-18, 1971*, **3**, 229-255 (1971).

**Key words:** Buckling; columns; creep; creep buckling; full-scale testing; load capacity; performance criteria; performance evaluation; performance testing; structural analysis; structural testing.

A major effort is now underway in the United States to introduce industrialized housing systems. This effort was initiated by the Department of Housing and Urban Development and is known as Operation Breakthrough. As a part of this effort, performance criteria were developed which make it possible to evaluate the structural adequacy of innovative systems. The criteria,

analysis, and testing with respect to creep buckling are discussed. A case history is presented of the evaluation of the structural adequacy with respect to creep buckling of an innovative reinforced concrete system. The system was evaluated by full-scale testing and by analysis. An analytical approach was developed to predict the adequacy of reinforced concrete structural systems with respect to creep buckling.

**12994.** Semmelroth, C. C., **Adjustment of the Munsell-value and W\*-scales to uniform lightness steps for various background reflectances**, *Appl. Opt.* **10**, No. 1, 14-18 (Jan. 1971).

**Key words:** Color; lightness; vision.

For background reflectances taken equal to, or slightly lower than, the specimen reflectances, the Munsell-value, *V*, and the CIE 1964, *W\**, scales are found to be essentially linear with a power formulation for lightness previously shown to accord with lightness-spacing data for a wide variety of specimen and background reflectances. Adjustments required to make the Munsell-value function accord precisely with the power formulation for this background condition are all less than 0.2 of a Munsell-value step between 1/ and 9/. The power formulation is used to construct a table to show in Munsell terms the influence of background reflectance on perceived lightness for all combinations of specimen and background reflectance including Takasaki crispening for specimen reflectance approaching that of the background.

**12995.** Ritter, J. J., Coyle, T. D., Bellama, J. M., **Reactions of tetrachlorodiborane (4) with fluoroolefins**, *J. Organometal Chem.* **42**, 25-31 (1972).

**Key words:** Boron; boron subhalides; fluoroolefins; halides; haloolefin; organoboron compounds; tetrachlorodiborane (4); tetrafluorodiborane (4).

Tetrachlorodiborane (4) reacts with trifluoroethylene to give dichloro-2,2-difluorovinylborane and both isomers of dichloro-2-chloro-2-fluorovinylborane. These compounds can be converted to the corresponding difluoro (halovinyl) boranes by treatment with SbF<sub>3</sub>. Reaction of B<sub>2</sub>Cl<sub>4</sub> with vinyl fluoride gives 1,1,2-tris (dichloroboryl) ethane. A facile halogen exchange with B<sub>2</sub>Cl<sub>4</sub> was observed for a number of fluoroolefins, including vinyl fluoride, 1,1-difluoroethylene, 2-fluoropropene, and 3,3,3-trifluoropropene. No reaction was observed with 2,3,3,3-tetrafluoropropene.

**12996.** Rebbert, R. E., Lias, S. G., Ausloos, P., **Vacuum ultraviolet photolysis of methane. Reaction of methylene**, *Chem. Phys. Lett.* **12**, No. 2, 323-326 (Dec. 15, 1971).

**Key words:** Deactivation; insertion reaction; lifetime; methane; methylene; photolysis; quantum yields.

Methylene radicals formed in the photolysis of methane (123.6 and 104.8–106.7 nm) insert into the C–H bond of methane to produce ethane molecules whose lifetime is independent of the energy of the photon. Deactivation of ethane by collision with methane is stepwise, and the lifetime of the insertion product is shorter than reported in previous CH<sub>3</sub>CO photolysis studies.

**12997.** deWit, R., **The relation between continuous and discrete disclinations**, (Proc. Int. Symp. on Foundations of Plasticity, Warsaw, Poland, Aug. 30-Sept. 2, 1972), *Arch. Mech.* **24**, No. 3, 499-510 (Wolters-Noordhoff Publ. Co., 1972).

**Key words:** Continuous; continuum; defect; disclination; discrete; dislocation; distortion; Green's function; incompatibility; plasticity; strain; Volterra.

A recent paper of Mura introduces plastic and elastic distortions to describe a theory of disclinations. Our objection to this

approach is that the "elastic distortion" is not a state quantity when disclinations are present. Mura's "plastic distortion" for a line singularity is examined in the light of our theory and found to represent a dislocation wall terminating inside the body on a dislocation loop. Mura's "plastic rotation" is found to represent a dislocation wall terminating on a disclination. The sum of these two gives the "disclination" loop. Explicit expressions are derived for the elastic strain and bend-twist in both the discrete and continuous cases, which show that, contrary to the "elastic distortion," they are indeed state quantities.

- 12998.** Forman, R. A., Brower, W. S., Jr., Parker, H. S., **Phonons and the green exciton series in cuprous oxide,  $\text{Cu}_2\text{O}$** , *Phys. Lett.* **36A**, No. 5, 395-396 (Sept. 27, 1971).

Key words: Copper oxide; cuprous oxide; excitons; forbidden bandgap; phonons.

Examination of the optical absorption edge spectra of samples of melt-grown cuprous oxide enables identification of features of the green exciton series overlying the yellow series. Identification of the green series  $n=1$  line allows new interpretations of various features seen earlier by other workers.

- 12999.** Sieck, L. W., Hellner, L., Gorden, R., Jr., **Kinetic mass spectrometric determination of the absolute rate coefficient for the reaction  $\text{NH}_3^+ (\nu=0) + \text{NH}_3 \rightarrow \text{NH}_4^+ + \text{NH}_2$  at thermal kinetic energies**, *Chem. Phys. Lett.* **10**, No. 5, 502-503 (Sept. 1, 1971).

Key words: Ammonia; mass spectrometry; photoionization; rate constants; thermal energy; vibrational energy.

The absolute thermal rate coefficient for the reaction  $\text{NH}_3^+ + \text{NH}_3 \rightarrow \text{NH}_4^+ + \text{NH}_2$  has been determined experimentally for the first time for  $\text{NH}_3^+ (\nu=0)$  reactant ions. An increase in  $E_{\text{vib}}$  results in a decrease in the rate coefficient for proton transfer.

- 13000.** Ausloos, P., **Far ultraviolet photolysis of alkanes**, *Mol. Photochem.* **4**, No. 1, 39-55 (1972).

Key words: Energy partitioning; energy transfer; excited states; fluorescence; photoionization; photolysis; quantum yields.

The effect of wavelength on the primary photophysical and photochemical processes is reviewed. Quantum yields of the photoionization and of the photochemical decomposition of selected alkanes are presented. The modes of dissociation of neutral electronically excited alkanes are related to information derived from high resolution gas phase absorption spectra and from liquid phase fluorescence measurements. The effect of phase on the primary decomposition mechanism and on energy transfer processes is examined in the light of recent findings. New experimental information on the energy partitioning among fragments produced in the primary dissociation of  $\text{CH}_4$  and  $\text{C}_3\text{H}_8$  is presented.

- 13001.** Mandel, J., **The statistical validation of tests**, *Mater. Res. Stand.* **12**, No. 9, 8-13.62 (Sept. 1972).

Key words: Experimental error; measurement; statistical control; statistical design; test methods.

Basic to the evaluation of test methods is an understanding of the behavior of measurements, and particularly of the disturbances caused by random and systematic experimental errors. The concept of statistical control is discussed in terms of measuring processes. Finally, the role of statistical models and designs is illustrated by an example dealing with certain physical characteristics of a blood expander.

- 13002.** Sieck, L. W., Ausloos, P., **Ion-molecule reaction chains in isobutene**, *J. Chem. Phys.* **56**, No. 2, 1010-1011 (Jan. 15, 1972).

Key words: Ion-molecule reactions; isobutene; photoionization; polymerization; radiolysis.

The vapor phase ionic-chain reaction occurring in isobutene and propylene have been investigated both in the NBS high pressure photoionization mass spectrometer and in the closed systems photolysis. We have determined for the first time that the formation of stable dimer ions  $(\text{C}_4\text{H}_8)_2^+$  in isobutene competes effectively with formation of  $\text{C}_4\text{H}_9^+$ . Dimeric ions are also observed in propylene. These dimeric ions are found to transfer  $\text{H}_2$  to isobutene and propylene to yield isobutane and propane, respectively. The failure of other investigators to observe these sequences is discussed.

- 13003.** Sieck, L. W., Searles, S. K., **High-pressure photoionization mass spectrometry. II. A study of thermal  $\text{H}^- (\text{H}^0)$  and  $\text{H}_2^- (\text{H}_2^0)$  transfer reactions occurring in alkane-olefin mixtures**, *J. Amer. Chem. Soc.* **92**, 10, 2937-2943 (May 20, 1970).

Key words: Alkanes; ion-molecule reactions; mass spectrometry; photoionization; rate coefficient; vapor phase.

Following photoionization of the  $\text{C}_n\text{H}_{2n}$  (olefin) or  $\text{RH}_2$  (alkane or cycloalkane) component in  $\text{RH}_2\text{-C}_n\text{H}_{2n}$  mixtures with either 1236-Å (10.0 eV) or 1165-Å (10.6 eV) radiation, the following two classes of reactions have been investigated: (I)  $\text{C}_n\text{H}_{2n}^+ + \text{RH}_2 \rightarrow \text{C}_n\text{H}_{2n+1}^+ + \text{RH}^+$  ( $\text{H}^-$  transfer) or  $\text{C}_n\text{H}_{2n+2}^+ + \text{R}^+$  ( $\text{H}_2^-$  transfer); (II)  $\text{RH}_2^+ + \text{C}_n\text{H}_{2n} \rightarrow \text{C}_n\text{H}_{2n+1}^+ + \text{RH}^+$  ( $\text{H}$  transfer) or  $\text{C}_n\text{H}_{2n+2}^+ + \text{R}^+$  ( $\text{H}_2$  transfer). Although these processes have been subjected to considerable scrutiny, the relative rate constants  $k(\text{H}^-)/k(\text{H}_2^-)$  or  $k(\text{H}^0)/k(\text{H}_2^0)$  found previously by kinetic mass spectrometry for any given reaction pair have always been considerably higher than those derived from photoionization and radiolysis experiments conducted in static systems. However, the values derived in our instrument, which reflect the interactions of ions at thermal energy, are in excellent agreement with the relative transfer efficiencies and other rate parameters derived from static experiments and suggest that kinetic and/or internal energy effects may have been important in previous experiments carried out in mass spectrometers. Rate constants and relative transfer efficiencies found for a number of reaction pairs are reported, and the nature of the collision complex is discussed.

- 13004.** McBee, C. L., Kruger, J., **Nature of passive films on iron-chromium alloys**, *Electrochim. Acta* **17**, 1337-1341 (Oct. 1972).

Key words: Amorphous; diffraction; Fe-Cr; lattice parameter; 1 N  $\text{H}_2\text{SO}_4$ ; oxide; passive; spinel.

Fe-Cr foils of a range of Cr content were anodically polarized in 1 N  $\text{H}_2\text{SO}_4$  for passive film growth. The resulting oxide films were then studied while still in contact with the metal substrate with transmission electron diffraction at 100 kV.

Comparisons were made between the diffraction results for the Fe-Cr foils and previous diffraction studies for Fe foils. The diffraction patterns obtained revealed that as Cr content increased the oxide films were generally less able to sustain an epitaxial relationship with the substrates. The lower Cr foils had oxide patterns that could be fitted to a spinel structure; the lattice parameter in these cases increased with increasing Cr content. The highest Cr-content alloy, Fe-24% Cr, did not show any oxide pattern. It is concluded that the films tend to become amorphous as the Cr content of the alloy is increased.

- 13005.** Sindt, C. F., Ludtke, P. R., **Characteristics of slush and boiling methane and methane mixtures**, *Proc. XIIIth Int. Con-*



gress of the International Institute of Refrigeration, Washington, D.C., Aug. 27-Sept. 3, 1971, pp. 1-6 (Int. Inst. of Refrigeration, Paris, France, 1971).

**Key words:** Binary mixtures; cryogenic mixtures; liquefied natural gas; methane; slush methane; slush natural gas.

Liquefied natural gas (LNG) and methane are in contention as fuels for high performance aircraft, rocket engines, and motor vehicles. They have the advantages, over kerosene and gasoline, of higher specific heat of combustion and cleaner combustion, and they are six times more dense than liquid hydrogen. Some of the applications for either methane or LNG would benefit from the increased heat capacity and the increased density of mixtures of liquid and solid such as slush. Because of these potential advantages, the characteristics of slush and boiling methane and binary mixtures of methane and other natural gas constituents were investigated. Subcooled liquid or slush would also serve to reduce or eliminate fuel losses that would accompany reduction in fuel tank pressure as the aircraft gains altitude.

The scope of the program was the characterization of slush prepared from pure methane and binary mixtures of methane with nitrogen, ethane, and propane, and the investigations of the boiling characteristics of these mixtures.

**13006.** Grabner, L., Forman, R. A., Wong, E. Y., **Spectroscopy of  $\text{Cr}^{3+}$  in  $\text{CsCr}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}/\text{D}_2\text{O}$ , a  $\beta$ -alum**, *Phys. Rev. B* 6, No. 3, 797-801 (Aug. 1, 1972).

**Key words:**  $\alpha$ -,  $\beta$ -,  $\gamma$ -alums; crystal field splitting; disorder; energy transfer; inequivalent sites.

The trigonal-field splitting of  ${}^2\bar{E}$  into  $\bar{E}$  and  $2\bar{A}$  states is found to be  $\bar{E} - 2\bar{A} = -120 \text{ cm}^{-1}$  by identifying  $2\bar{A}$ . The no-phonon lines of deuterated samples are isotope shifted  $6 \text{ cm}^{-1}$  to the red. The following generalizations suffice to relate the spectra of the Cr-alums: (i) They are due to  ${}^4A_2 \rightarrow \bar{E}$ ,  $2\bar{A}({}^2E)$  transitions. The splitting of  ${}^2E$  is large for the  $\beta$ -alums, small for the  $\alpha$ -alums. (ii) Sulfate-group disorder, found in all  $\alpha$ -alums, complicates their spectra by adding inequivalent  $\text{Cr}^{3+}$  sites.

**13007.** Frederikse, H. P. R., Hosler, W. R., **Excitons in solid and liquid thallous chloride**, *Solid State Commun.* 9, No. 10, 709-712 (1971).

**Key words:** Excitons; liquid state; thallous chloride.

The absorption edge of thallous chloride has been measured below and above melting point. In the crystal this edge represents the low energy tail of a strongly absorbing Wannier exciton. The similarity between the shape and temperature dependence of this absorption in the solid and in the liquid states suggests that Wannier-like excitons exist also in liquid thallous chloride.

**13008.** Grabner, L., **Exciton emission and donor-acceptor association in thallium bromide**, *Phys. Rev. B* 4, No. 4, 1335-1339 (Aug. 15, 1971).

**Key words:** Donor-acceptor pairs; excitons; thallium bromide.

Free- and bound-exciton emission with longitudinal optical (LO) phonon cooperation is reported in undoped TlBr. The binding energies of the bound excitons with respect to the free exciton are 4 and 7 MeV, respectively. A photocurrent peak at the energy of the free exciton at 4 K is interpreted as due to an Auger process at the bound-exciton complexes. Extrinsic photocurrent is reported. The temperature dependence of its excitation spectrum is anomalous from the point of view of the conventional Riehl-Schön recombination model and is shown to be consistent with a model involving donor-acceptor pairs.

**13009.** Forman, R. A., **Order-disorder transition in lithium imide,  $\text{Li}_2\text{NH}$** , *J. Chem. Phys. Letters to Editor* 55, No. 4, 1987-1988 (Aug. 15, 1971).

**Key words:** Dipole ordering; DTA; NMR; order-disorder; phase transition; thermal analysis.

On the basis of differential thermal analysis results and previous NMR studies, we believe we have discovered an order-disorder transition, possibly of the  $\lambda$ -type, of  $\text{NH}_2^-$  dipoles in the cubic anti-fluorite compound lithium imide,  $\text{Li}_2\text{NH}$ .

**13010.** Franzen, D. L., **CW gas breakdown in argon using 10.6- $\mu\text{m}$  laser radiation**, *Appl. Phys. Lett.* 21, No. 2, 62-64 (July 15, 1972).

**Key words:** Gas breakdown; plasma.

A very intense gas breakdown spark has been extended to a continuous arc in argon using a focused cw  $\text{CO}_2$  laser. To achieve cw breakdown, the focal volume of a mirror focusing a high-power  $\text{CO}_2$  laser was preionized by a single pulse from a  $\text{CO}_2$  TEA laser. The electron density created by the pulsed laser is sufficient to start the cw plasma. This letter reports accurate measurements of pulsed thresholds as well as preionized cw thresholds for breakdown in argon. Also, a study of the time development of the cw plasma is presented.

**13011.** Hedges, R. E. M., Drummond, D. L., Gallagher, A., **Extreme-wing line broadening and Cs-inert-gas potentials**, *Phys. Rev. A* 6, No. 4, 1519-1544 (Oct. 1972).

**Key words:** Cesium; inert gas; line broadening; molecules.

The emission profiles of the cesium resonance lines broadened by collisions with inert gases have been measured from about  $50\text{--}1000 \text{ cm}^{-1}$  from line center. The emission is observed from optically excited Cs in a cell whose temperature is varied from about  $300\text{--}800 \text{ K}$ . By measuring the wing intensity relative to the entire line intensity from optically thin Cs, the profiles can be related to theoretical models without knowledge of the cesium density. The quasistatic theory of line broadening, extended to include the distribution of perturber positions about the Cs, is used to analyze the data. The observed temperature dependence of the emission profiles is associated with the temperature dependence of the perturber distribution in the Cs-inert-gas adiabatic potential. The quasistatic spectrum depends on the difference between excited- and ground-state adiabatic potentials, so each potential is thereby separately determined from the data. The  $X\Sigma$ ,  $A\Pi$ , and  $B\Sigma$  potentials for the  $3.5\text{--}5\text{-}\text{\AA}$  region are given.

**13012.** Kitching, P., Moss, G. A., Olsen, W. C., Roberts, W. J., Alder, J. C., Dollhopf, W., Kossler, W. J., Perdrisat, C. F., Lehman, D. R., Priest, J. R., **Reactions ( $p, pd$ ) and ( $p, 2p$ ) on helium-3 at 590 MeV**, *Phys. Rev. C* 6, No. 3, 769-772 (Sept. 1972).

**Key words:** Confidence cross sections;  ${}^3\text{He}(pd)$  vertex; plane wave impulse approximations; quasi-free scattering; separable potentials; three-body problem.

The reaction  ${}^3\text{He}(p, pd)$  has been studied for recoil momenta of the spectator proton up to  $230 \text{ MeV}/c$ . The cross section of  ${}^3\text{He}(p, 2p)$  was measured up to  $100 \text{ MeV}/c$ . The results are interpreted in terms of the plane-wave impulse approximation and the form factors for  ${}^3\text{He} \rightarrow dp$  and  ${}^3\text{He} \rightarrow p(pn)$  are compared with a calculation of the  ${}^3\text{He}$  wave function in which the two-nucleon interaction is described by a separable potential which reproduces the low-energy properties of the two-nucleon system.

**13013.** Markus, W., **A constant volume valve**, *Rev. Sci. Instrum. Notes* 43, No. 1, 158-159 (Jan. 1972).

**Key words:** Constant volume; equation of state; pressure; vacuum; valve.

A constant volume valve is described for pressures to 1400 bar with a volume change between the open and closed positions of less than  $0.15 \text{ mm}^3$ . The leak rate through the seat is less than  $5 \times 10^{-5}$  mole/sec. The valve is of a very simple design. The type described here is pneumatically operated.

- 13014.** Cohen, M. I., Young, K. F., Chang, T-T., Brower, W. S., Jr., **Phase transitions in  $\text{CsPbCl}_3$** , *J. Appl. Phys.* **42**, No. 13, 5267-5272 (Dec. 1971).

Key words:  $\text{CsPbCl}_3$ ; EPR of  $\text{Gd}^{3+}$ ; phase transitions.

Measurements of dielectric properties, pyroelectricity, and the electron paramagnetic resonance spectrum of  $\text{Gd}^{3+}$  as a function of temperature have been used to examine the phase transitions in  $\text{CsPbCl}_3$ . The results indicate the presence of five phase transitions and the loss of a center of symmetry at 194 K. The results together with the apparent order of the transitions, and published data, enable the Landau criterion to be used so that the point group of each phase may be identified. A reasonable choice of space group is also made.

- 13015.** Forman, R. A., Brower, W. S., Jr., **Optical spectra of thallium-doped ammonium chloride**, *J. Lumin.* **4**, No. 2, 98-104 (Sept. 1971).

Key words: Ammonium chloride; luminescence, optical absorption; optical spectra; thallium ion.

The low temperature optical spectra associated with the thallium ion in doped samples of ammonium chloride have been investigated. Absorption, photoluminescence and luminescence excitation spectra are presented for this  $\text{CsCl}$ -structure (cubic) phosphor.

- 13016.** Feldman, A., Horowitz, D., Waxler, R. M., **Relative importance of electrostriction and the Kerr effect to self-focusing in optical glasses**, *Appl. Phys. Lett.* **21**, No. 6, 260-262 (Sept. 15, 1972).

Key words: Damage threshold; electrostriction; Kerr-effect; laser damage in glasses; optical glasses; self-focusing.

The damage threshold for three optical glasses was found to be higher for circularly polarized radiation than for linear polarization, using 26-nsec pulses from a Nd:glass laser. The damage was assumed to result from self-focusing. The fractional contribution of electrostriction to the total nonlinear index  $n_2$  is estimated to be  $0.8 \pm 0.2$  for borosilicate crown glass,  $1.15 \pm 0.35$  for fused silica, and  $0.4 \pm 0.1$  for dense flint glass, assuming the Kerr effect to be the only other self-focusing mechanism. The data are consistent with present concepts of glass structure. The high damage threshold in fused silica is attributed to its relatively small Kerr effect.

- 13017.** Forman, R. A., Hosler, W. R., Blunt, R. F., **The bandgap of cadmium fluoride**, *Solid State Commun.* **10**, No. 1, 19-24 (1972).

Key words: Bandgap; band structure; cadmium fluoride excitons; optical absorption; reflectivity; semiconductor.

Measurements of optical absorption and reflection at and below room temperature have been used to indicate that cadmium fluoride is a direct allowed bandgap material. In absorption an Urbach-type edge is observed, with the extrapolations from various temperatures intersecting to indicate an excitonic bandedge of  $\sim 7.6 \text{ eV}$  in agreement with the reflectivity data. The absorption data are in accord with the thermal behavior expected for an allowed excitonic transition.

- 13018.** Mandel, J., **Principal components, analysis of variance and data structure**, *Statist. Neerlandica*, pp. 119-129 (Aug. 1972).

Key words: Analysis of variance; data structure; principal components; two-factor data.

The relation between principal components and analysis of variance is examined. It is shown that the model underlying the extended analysis of variance developed by GOLLOB and MANDEL is useful also as a model for principal component analysis. The elucidation of structure of two-factor data using the new analysis of variance model is illustrated by an example taken from thermodynamics.

- 13019.** Kraft, R., **Analyticity and reflectivity for first order systems of elliptic type in two independent variables**, *J. Math. Anal. Appl.* **29**, No. 1, 1-17 (Jan. 1970).

Key words: Analytic continuation; analyticity; complex variables; elliptic type; first order systems; partial differential equations; semilinear.

Analyticity and reflectivity results are established for first order elliptic semilinear systems in two independent variables. The results are obtained by adaption and modifications of techniques used by Garabedian in establishing similar results for second order systems.

- 13020.** Rockett, J. A., **Fire research and safety center and the fire marshal**, *Fire J.* **64**, No. 6, 50-53 (Nov. 1970).

Key words: Education; fire act; fire data; fire prevention; fire protection; training.

The present status of the Fire Research and Safety program is discussed. Programs which will be of particular interest to the Fire Marshal are described. These include assistance in: fire records; fire record management and the use of fire data; fire investigations; training and education.

- 13021.** Dillon, T. A., Stephenson, J. C., **Multiquantum vibrational-energy exchange**, *Phys. Rev. A* **6**, No. 4, 1460-1468 (Oct. 1972).

Key words: Born; CO; collisions; exchange; multiquantum.

A theory for exchange of vibrational quanta between molecules is formulated which does not rely on the Born expansion of the  $S$  matrix. A transformation is derived which diagonalizes the vibrational operators responsible for exchange. The scattering operator is then expanded in a series of rotational tensor operators which permits evaluation of  $S$ -matrix elements to all orders. This formulation shows that multiquantum processes, both rotational and vibrational, play an important role when transition moments are large. Numerical calculations for vibrational exchange rates of carbon monoxide are compared with results of the first Born approximation from which they differ significantly. The dependence of the cross section on vibrational-energy defect is much less drastic than that of the Born approximation. The present calculations indicate that cross sections for the exchange of more than one vibrational quantum are substantial, in marked contrast to the Born approximation where they are forbidden. The size of these multiquantum cross sections indicates that they can play an important role in the detailed kinetic modeling of CO lasers.

- 13022.** Harman, G. G., Leedy, K. O., **An experimental model of the microelectronic ultrasonic wire bonding mechanism**, *Proc. 10th Annual IEEE Reliability Physics Symposium, Las Vegas, Nevada, Apr. 5-7, 1972*, pp. 49-56 (1972).

Key words: Aluminum; microelectronics; ultrasonic bonding; wire bonding.

Various concepts of the microelectronic ultrasonic bonding mechanism have been expounded for many years. The present work attempts to resolve some of the conflicts by experimentally



examining each step in the ultrasonic aluminum wire bonding process. Measurements made with a capacitor microphone during bonding are correlated with appropriate SEM pictures of bond lift-off patterns. A series of inductive experiments have been performed, the results of which can be summarized as follows: Heat generation in the weldments is insufficient to cause the observed welding. The deforming wire breaks up and sweeps aside oxide, exposing clean metal surfaces which are then able to form metallurgical welds. The bonding tool does not grip the wire and slide it back and forth across the bonding pad. The use of a grooved tool does not improve the welding process. The tool-to-wire coupling takes place by a series of microwelds that are repeatedly made and broken as the tool moves back and forth across the wire surface.

**13023.** Bennett, H. S., Stoneham, A. M., **Effects of random fields on radiative decay of color centers**, *Phys. Rev. B* **6**, No. 8, 3086-3090 (Oct. 15, 1972).

Key words: Charged impurities; *F* center; Gaussian distribution; Holtsmark distributions; lifetime; phonons; potassium chloride.

Transitions which are normally forbidden have been observed in a variety of defects in solids because of the electric fields associated with lattice vibrations or with random impurities. The radiative decay of an *F* center is a good example of this. We ask in this paper: When will the contribution of random impurities be important, and when will the decay be intrinsic? Several qualitatively distinct examples are analyzed, and tables for the transition probabilities in terms of dimensionless parameters characteristic of the host and the defects are given. Random fields should dominate in III-V and group-IV hosts, but they should prove less important in the alkali halides. Effects of random fields on related phenomena are also discussed.

**13024.** Baker, L. C. W., Baker, V. S., Wasfi, S. H., Candela, G. A., Kahn, A. H., **Isomorphous heteropoly complexes containing various pairs of paramagnetic atoms. Exchange-coupled differing spins with absence of long-range magnetic interactions. A new class of paramagnetic behavior. Theoretical treatment. Novel geometrical isomerism**, *J. Amer. Chem. Soc.* **94**, No. 15, 5499-5501 (July 26, 1972).

Key words: CO; exchange coupling; Fe; heteropoly complexes; Keggin structures; magnetic spins; magnetic susceptibility; paired spins; tungsto-heteropoly complexes.

Coupled pairs of differing magnetic ions in tungsto-heteropoly complexes have been studied by magnetic susceptibility over the temperature range 2 to 300 K. The two substitutional sites are surrounded by oxygen ions in octahedral and tetrahedral coordinations with one oxygen ion in common. The ions studied were  $\text{Co}^{2+}$ ,  $\text{Co}^{3+}$ , and  $\text{Fe}^{3+}$ , in a total of five combinations on the two sites, offering a unique set of symmetries and ions for examining super-exchange effects. The susceptibility has been analyzed according to the spin Hamiltonian

$$\mathcal{H} = \beta(g_1 S_1 + g_2 S_2) \cdot \mathbf{H} - JS_1 \cdot S_2;$$

fitted values of *J* range from -6 to -70 K depending on the combinations of ions. The experimental agreement with the spin Hamiltonian for all cases studied is satisfactory for this unique system.

**13025.** Linsky, J. L., Mount, G. H., **On the validity of a generalized Kirchhoff's Law for a nonisothermal scattering and absorptive medium**, *Icarus* **17**, 193-197 (1972).

Key words: Emissivity; Kirchhoff's Law; lunar surfaces; planetary atmospheres; reflectivity.

The relationship of directional hemispherical reflectivity to emissivity is investigated for a nonisothermal medium with isotropic coherent scattering and absorption. Departures from a generalized Kirchhoff's Law occur due to the long range nature of the scattering process. Such departures occur in lunar thermal emission at microwave but not at infrared frequencies.

**13026.** Trombka, J. I., Eller, E., Oswald, G. A., Berger, M. J., Seltzer, S. M., **<sup>252</sup>Cf neutron induced radiative capture gamma rays for high energy detector calibration**, (Proc. Amer. Nucl. Soc. National Topical Meeting on Neutron Sources and Applications, Augusta, Ga., April 19-21, 1971), Chapter in *Neutron Sources and Applications*, CONF-710402, 111, 111-43-III-47 (National Technical Information Service, Springfield, Va. 22151, 1971).

Key words: California; gamma rays; neutrons; radiative capture; response functions; sodium iodide detector.

High energy gamma ray sources produced by prompt neutron radiative capture were developed in order to study the variation of pulse height, the shape of pulse height distribution, and resolution as a function of energy for scintillation detectors. The system as described below has also been used to calibrate the gamma ray spectrometers which will be flown aboard Apollo 15 and 16.

Spectral distribution of gamma rays in the 3 to 12 MeV energy region using a 3 in. x 3 in. NaI(Tl) detector have been studied for a number of nuclear species such as: Nickel with lines at 8.999 and 8.533 MeV; Mercury-5.967, 4.842, 4.740, and 3.289 MeV; and Hydrogen-2.223 MeV. The neutron excitation of these samples was carried out by placing these samples in a neutron moderator near a <sup>252</sup>Cf source (~2 μg).

Methods for inferring photon spectra from the pulse height spectra have been developed and are to be used to interpret the gamma ray measurements carried out during the Apollo 15 and 16 flights. Detailed knowledge of the response of the flight detectors as a function of energy is required to perform the analysis. In the energy region above 3 MeV, it is extremely difficult to obtain response functions for truly monoenergetic gamma rays. Therefore the following approach has been taken: Monte Carlo calculations have been carried out to determine the nature of these response functions in the 3 to 12 MeV region. These spectra have been compared with the experimentally determined spectra obtained using the <sup>252</sup>Cf system described above. These comparisons form a basis for predicting the shape of the pulse height spectrum for gamma rays of any energy in this range.

**13027.** Cowan, D. O., Candela, G. A., Kaufman, F., **The organic solid state. V. Symmetry distortions in ferrocenium compounds**, *J. Amer. Chem. Soc.* **93**, No. 16, 3889-3893 (Aug. 11, 1971).

Key words: Biferrocene; electron resonance; susceptibility; symmetry changes.

The magnetic susceptibilities of biferrocene [ $\text{Fe(II)Fe(III)}$ ] picrate (1) and biferrocene [ $\text{Fe(II)Fe(III)}$ ] difluoroborate (2) were determined from 2 to 300 K. The experimental curves for the effective magnetic moment ( $\mu_{\text{eff}}$ ) are compared with theoretical curves based on a model involving molecular distortion from axial symmetry. For compound 1, in the temperature range 77-300 K, the best-fit temperature-independent distortion factor ( $\delta = 1000 \text{ cm}^{-1}/\text{ferrocenium unit}$ ) is large when compared to previously observed distortions. The deviation from the theoretical  $\mu_{\text{eff}}$  curve for this compound is small. For compound 2 in the temperature range 77-300 K the best-fit temperature-independent distortion factor is  $750 \text{ cm}^{-1}/\text{ferrocenium unit}$ ; while in the temperature range 2-4 K the distortion factor is considerably smaller ( $\delta = 150 \text{ cm}^{-1}/\text{ferrocenium unit}$ ). The electron spin resonance spectra of compounds 1 and 2 were measured at 77



and 298 K. The observed  $g$  values were used to calculate the effective magnetic moments and the distortion factors for compounds 1 and 2. These values are in good agreement with those obtained from the magnetic susceptibility measurements. The observed low-temperature collapse of the  $g_x$ ,  $g_y$  signal and the appearance of a new  $g_z$  signal (compound 2) are consistent with a large reduction in the distortion parameter at low temperature.

**13028.** Wacławski, B. J., Plummer, E. W., **Photoemission observation of a surface state of tungsten**, *Phys. Rev. Lett.* **29**, No. 12, 783-786 (Sept. 1972).

**Key words:** Adsorption; energy distribution; photoemission; surface states.

Photoelectron energy distributions from clean, polycrystalline tungsten reveal a surface-sensitive peak about 0.4 eV below the Fermi energy. This peak, which is identified as a surface state, rapidly decays during gas adsorption, and concomitant growth of a new peak at  $\sim 2.5$  eV below the Fermi energy is observed. Over the energy range of the surface-state peak, the strength of surface-state emission relative to bulk emission decreases with increasing photon energy. These results quantitatively substantiate existing field-emission data and qualitatively agree with model photoemission calculations.

**13029.** Steiner, B., **Photodetachment: Cross sections and electron affinities**, Chapter 7 in *Case Studies in Atomic Collision Physics*, E. W. McDaniel and M. R. C. McDowell, Eds., **2**, 485-545 (North-Holland Publ. Co., Amsterdam, The Netherlands, 1972).

**Key words:** Atomic; crossed beam; cross section; electron affinity; molecular; photodetachment.

The status of negative ion photodetachment cross section determination is reviewed, both theory and experiment. A selected table of best values is derived. Threshold behavior is examined separately. Crossed beam experimental techniques are described in detail. Finally, the status of atomic and molecular electron affinity determinations is reviewed and an extensive table of preferred values is compiled.

**13030.** Nargolwalla, S. S., **Application of neutron generators to activation analysis**, (Proc. Second Oak Ridge Conf. on the Use of Small Accelerators for Teaching and Research, Oak Ridge, Tenn., Mar. 23-25, 1970), USAEC Rept. Conf. 700322, 185-204 (Oct. 1970).

**Key words:** Accuracy; activation analysis; element; generator; micro; precision; reactor; selectivity; semimicro; sensitivity.

Neutron activation analysis has gained wide acceptance in recent years as a very sensitive and specific method for the qualitative and quantitative determination of most of the elements in the periodic table. Until very recently, however, activation analysis was limited to the use of thermal neutrons generated in a nuclear reactor. Today, the development of low-cost neutron generators has considerably added to the scope of the technique, and made it available to most well-equipped analytical laboratories. This review summarizes some of the key developments in neutron generator technology which have had a significant bearing in the acceptance of neutron generators for the precise and accurate determination of a large number of elements at the semimicro and macro levels of concentration.

Recent advances in the design and utilization of experimental hardware such as sample-placement devices, experimental designs and special long-lived neutron producing targets are discussed. Descriptions of some investigations pertaining to the evaluation of systematic errors in activation analysis with neutron generators are presented, and various aspects of analytical

significance related to the use of this type of radiation source are emphasized. In this regard, advantages offered by the neutron generator for the analysis of light elements are given. Research in the area of cross section measurements and their implications in light of the practical sample due to degradation of the nominal 14.7 MeV neutrons is described. Typical sensitivities obtainable with present-day neutron outputs from neutron generators are critically examined and anomalies between expected theoretical sensitivities and experimental sample response in high energy neutrons are discussed.

Pertinent applications of neutron generator activation analysis techniques in the areas of metallurgy, biochemistry, mineralogy and standard materials are described. Special attention is drawn to the introduction of this technique to the solution of industrial quality control problems. A brief treatment of the on-line analytical capabilities of neutron generators, particularly of the sealed-tube type is given. In this connection, efforts made toward the computerization of analytical procedures and data reduction are emphasized. In conclusion, the contribution of this analytical technique in terms of sensitivity, specificity, accuracy and precision, and possible future developments of the fast neutron facility are discussed.

**13031.** Baker, L. C. W., Baker, V. E. S., Wasfi, S. H., Candela, G. A., Kahn, A. H., **Exchange interactions between pairs of differing magnetic spins in heteropoly complexes**, *J. Chem. Phys.* **56**, No. 10, 4917-4923 (May 15, 1972).

**Key words:** Co; Fe; heteropoly complexes; Keggin structures; magnetic spins; magnetic susceptibility; paired spins; tungsto-heteropoly complexes.

Coupled pairs of differing magnetic spins in tungsto-heteropoly complexes have been investigated by studying the magnetic susceptibility over the temperature range 2-300 K. The two sites of the magnetic ions are surrounded by oxygen ions in octahedral and tetrahedral coordinations with one oxygen ion in common. The ions studied were  $\text{Co}^{2+}$ ,  $\text{Co}^{3+}$ , and  $\text{Fe}^{3+}$  in a total of six combinations on the two sites, offering a unique set of symmetries and ions for examining super-exchange effects. A closed form for the susceptibility has been obtained on assuming the spin Hamiltonian

$$\mathcal{H} = \beta(g_1 S_1 + g_2 S_2) H - JS_1 \cdot S_2,$$

allowing for the possibility of  $g_1 \neq g_2$ ,  $S_1 \neq S_2$ . Fitted values of  $J/k$  range from  $-6$  to  $-70$  K depending on the combination of ions. The experimental agreement with the spin Hamiltonian for all cases studied is satisfactory for this system.

**13032.** McAlister, A. J., Cuthill, J. R., Dobbyn, R. C., Williams, M. L., Watson, R. E., **Soft-x-ray studies of ferromagnetic and paramagnetic iron**, *Phys. Rev. Lett.* **29**, No. 3, 179-182 (July 17, 1972).

**Key words:** Band ferromagnetism; Fe; magnetic transition; M spectrum; soft-x-ray.

The soft-x-ray  $M_{2,3}$  emission spectrum of Fe has been measured below ( $560^\circ\text{C}$ ,  $T/T_c = 0.8$ ) and above ( $840^\circ\text{C}$ ,  $T/T_c = 1.07$ ) the Curie point, and has revealed motion of distinct structural features within the  $d$  bands on passing through  $T_c$ . The results, taken with earlier photoemission data on Fe and Ni, are in excellent numerical agreement with, while in no sense providing verification of, the band ferromagnetism description of Stoner, Wohlfarth, and Slater for these metals.

**13033.** Reno, R. C., Swartzendruber, L. J., **Time-differential perturbed angular correlations on  $^{57}\text{Fe}$  in Cu-Ni alloys: Mössbauer doublets explained**, *Phys. Rev. Lett.* **29**, No. 11, 712-715 (Sept. 11, 1972).



**Key words:** Cu-Ni-Fe alloys; hyperfine fields; Mössbauer effect; perturbed angular correlation.

It is shown that when hyperfine interactions at  $^{57}\text{Fe}$  nuclei are studied by both Mössbauer effect and time-differential perturbed angular correlations, information is obtained which is unavailable from either technique alone. In particular, previous ambiguities in the interpretation of  $^{57}\text{Fe}$  Mössbauer spectra of Cu-Ni alloys are removed: The Mössbauer doublet is shown to be primarily due to a distribution of electric field gradients acting on the  $^{57}\text{Fe}$  nuclei.

- 13034.** Nahman, N. S., Holt, D. R., **Transient analysis of coaxial cables using the skin effect approximation  $A=B\sqrt{s}$ , *IEEE Trans. Circuit Theory* CT-19, No. 5, 443-451 (Sept. 1972).**

**Key words:** Analysis; cables; coaxial; skin effect; time-domain; transient; transmission.

The purpose of this paper is to demonstrate the utility of the function  $A+B\sqrt{s}$  for approximating the coaxial line series impedance (skin effect) in applications to transient analysis. The time domain response expansions of Holt are modified in terms of two adjustable parameters which replace the physical parameters  $R$  and  $K$ . The modified expansions are truncated to yield condensed expressions useful for analysis and design. Two types of terminations are considered: 1) nonreflective, terminated in the characteristic impedance  $Z_0(s)$ , and 2) doubly reflective, sending and receiving ends each terminated in the nominal characteristic impedance  $R_0=\lim_{s\rightarrow\infty}Z_0(s)=\sqrt{L/C}$ . Experimental data are presented on the frequency and time domain insertion responses of three commercial cables: RG 5B/U—68.6 m (225 ft), RG 21/U—96.8 m (317 ft), and RG 58A/U—137 m (450 ft). Theoretical and experimental time domain responses for the sending- and receiving-end voltages are compared over the time interval from the order of 10 ns to that of 10  $\mu\text{s}$ . It is demonstrated that the parameters  $A$  and  $B$  can be adjusted to provide functions of time which closely approximate the actual time domain response over different intervals.

- 13035.** Barrow, L. E., **The mass-weight dilemma, *Sci. Teacher* 39, No. 7, 4 (Oct. 1972).**

**Key words:** Free fall; gravity; mass vs. weight; weight; weightlessness; weight vs. mass.

The impending changeover to the metric system has again given prominence to the confusion that exists regarding what the term "weight" signifies. This term for centuries has been used synonymously with mass but it has also been used to signify many other concepts, each related to the force of gravitational attraction in some way. The multiplicity of meanings of the term "weight" has created a dilemma the suggested resolution of which is the use of the term exclusively as being synonymous with mass and to use the term force when discussing any of the concepts related to gravity. How to handle the popularized concept of "weightlessness" is dealt with separately.

- 13036.** Ledbetter, H. M., Wayman, C. M., **On  $\beta$  AuCd martensites, *Met. Trans.* 3, No. 9, 2349-2356 (Sept. 1972).**

**Key words:** Crystallography; crystal structure/alloys; gold-cadmium alloys; phase transformations/solid state; x-ray-diffraction crystallography.

The martensites which form from  $\beta$  AuCd alloys have been studied by x-ray diffraction using both powder and single-crystal techniques. Alloys containing 46.8 to 51.0 at.pct Cd were examined. Besides the parent phase  $\beta$  only two other phases were observed:  $\beta'$  and  $\beta''$ . A new unit cell is proposed for  $\beta''$  which has 18 atoms and trigonal-hexagonal point symmetry. All previous  $\beta''$  crystal structure proposals are reviewed critically. The rela-

tionship of the  $\beta''$  crystal structure to the  $\beta$ -to- $\beta''$  martensitic transition is discussed.

- 13037.** Kirby, R. K., Hahn, T. A., Rothrock, B. D., **Thermal expansion, Section 4f in *American Institute of Physics Handbook, Third Ed.*, pp. 4-119-4-142 (1972).**

**Key words:** Alloys; compounds; elements; Grüneisen's constant; linear thermal expansion; liquids.

New and revised tables for the 3d edition of the AIP Handbook. These tables are: Table TE-1, Linear Thermal Expansion and Coefficients of Linear Thermal Expansion of Chemical Elements; Table TE-2, Coefficients of Linear Thermal Expansion of Materials at Low Temperatures; Table TE-3, Linear Thermal Expansion and Coefficients of Linear Thermal Expansion of Some Compounds and Alloys; Table TE-4, Thermal Expansion of Liquids; and Table TE-5, Constants in Grüneisen's Equation for Thermal Expansion (eight of the elements have been deleted from this table as it appeared in the 2d edition because the information is not consistent with the data given in TE-1).

- 13038.** Reed, R. P., **Aluminium. 2. A review of deformation properties of high purity aluminium and dilute aluminium alloys, *Cryogenics* 12, No. 4, 259-291 (Aug. 1972).**

**Key words:** Elastic properties; high-purity aluminium; lattice defects; mechanical properties; recovery; strengthening.

The elastic and plastic deformation behaviour of high-purity aluminium and of dilute aluminium alloys is reviewed. Reliable property data, including elastic moduli, elastic coefficients, tensile, creep, fatigue, hardness, and impact are presented. Single crystal tensile results are discussed. Rather comprehensive reference lists, containing publications of the past 20 years, are included for each of the above categories. Defect structures and mechanisms responsible for mechanical behaviour are presented. Strengthening techniques (alloys, cold work, irradiation, quenching, composites) and recovery are briefly reviewed.

- 13039.** Clark, A. F., **Combination of a power transmission line and an active track for a magnetically suspended high-speed train, *J. Appl. Phys.* 43, No. 8, 3598-3599 (Aug. 1972).**

**Key words:** Cryogenic; high-speed ground transportation; magnetic levitation; power transmission.

The idea of utilizing proposed cryogenic power transmission lines as an active track for magnetically suspended high-speed ground transportation is briefly explored. The advantages of transporting both people and power on the same right of way are many, and proposed transmission current levels are more than adequate for suspension.

- 13040.** Hanley, H. J. M., McCarty, R. D., **Argon third virial coefficients, *J. Chem. Phys.* 57, No. 7, 3023-3025 (Oct. 1, 1972).**

**Key words:** Argon; m-6-8 potential; nonadditivity; third virial coefficients.

Experimental third virial coefficients for argon, taken from several sources, are presented. An approximate calculation for the third virial coefficient from the 11-6-8 potential, including nonadditivity effects, is also discussed and the result compared to experiment. Agreement between theory and experiment is good.

- 13041.** Straty, G. C., Younglove, B. A., **Dielectric constant and molar polarizability of compressed gaseous and liquid fluorine, *J. Chem. Phys.* 57, No. 6, 2255-2259 (Sept. 15, 1972).**

**Key words:** Clausius-Mossotti function; compressed liquid; dielectric constant; fluorine; polarizability; saturated liquid.

In this paper we present accurate wide-range measurements of the dielectric constant of saturated liquid fluorine from 70 to 140 K and of compressed fluid fluorine at temperatures between 100 and 300 K at pressures to 21 MN/m<sup>2</sup> (1 MN/m<sup>2</sup> = 9.8692 atm = 145.038 psi). The data are combined with previously measured densities to determine the molar polarizability and its dependence on density and temperature. The density range examined extends to nearly 3 times the critical density. The molar polarizability is found to increase initially with density and then decrease. Current theories of the dielectric constant are found to give satisfactory qualitative interpretation of the density dependence of the molar polarizability but do not give satisfactory quantitative predictions.

**13042.** Hust, J. G., **Electrical resistance ratios of Evanohm heater wire at low temperatures**, *Rev. Sci. Instrum.* **43**, No. 9, 1387-1388 (Sept. 1972).

Key words: Electrical resistance; electrical resistance temperature coefficient; heater wire; material variability.

As a consequence of using Evanohm wire as heater elements in our thermal conductivity apparatus we have obtained extensive resistance-temperature data for wires from several spools at temperatures from 5 to 300 K. These data, reduced to resistance ratios,  $R(T)/R(273\text{ K})$ , show the variation of resistance with temperature as well as the degree of material variability.

**13043.** Berger, M. J., Seltzer, S. M., **Response functions for sodium iodide scintillation detectors**, *Nucl. Instrum. Methods* **104**, 317-332 (1972).

Key words: Detection efficiency; energy deposition spectrum; gamma ray spectrum; Monte Carlo calculations; resolution; response function; sodium iodide detector.

The response of sodium iodide detectors to gamma rays has been calculated by a method that takes into account the multiple scattering and escape from the detector of the incident gamma rays as well as of the secondary charged particles and bremsstrahlung. The method is applicable to gamma rays with arbitrarily high energies, and its accuracy has been verified by comparisons with experimental response functions at energies up to 20 MeV. A systematic tabulation has been made of the response functions for 3"×3" detectors irradiated with broad parallel beams of gamma rays, at energies between 100 keV and 20 MeV. These results are given in a parametrized form which makes it easy to interpolate with respect to incident gamma-ray energy. A few response functions have also been calculated for detectors irradiated with 50 MeV gamma rays. Exploratory calculations have shown that 3"×3" detectors are "omnidirectional" in the sense that the shape of the response function depends very little on the direction of the incident gamma-ray beam. Therefore, the tabulated data for broad parallel beams incident perpendicularly can, in good approximation, also be applied to other source geometries, e.g., the case of a detector exposed to an isotropic gamma-ray flux.

**13044.** Mielenz, K. D., Eckerle, K. L., **Spectrophotometer linearity testing using the double-aperture method**, *Appl. Opt.* **11**, No. 10, 2294-2303 (Oct. 1972).

Key words: Double-aperture method; light addition; non-linearity correction; photomultiplier nonlinearity; spectrophotometry.

The double-aperture method has been used to determine the nonlinearity correction for a new spectrophotometer having a precision of  $\pm 4 \times 10^{-5}$  transmittance units. The random and systematic errors of the method are discussed, and techniques are described that yield the additive nonlinearity correction to the high level of precision required for this spectrophotometer.

The correction was found to be independent of source polarization, free from interference errors, but slightly dependent on wavelength.

**13045.** Sugar, J., **Interpretation of photoabsorption in the vicinity of the 3d edges in La, Er, and Tm**, *Phys. Rev. A* **6**, No. 5, 1764-1767 (Nov. 1972).

Key words: Erbium; photoabsorption; theory; thulium; 3d edges.

Line spectra at the 3d photoabsorption edges of La, Er, and Tm are interpreted as transitions of the type  $3d^{10}4f^N \rightarrow 3d^9 4f^{N+1}$ . Calculated relative  $gf$  values for these transitions are compared with published absorption curves.

**13046.** Buchalter, D. N., Hargreaves, J. H., Jr., **Angular displacement detector**, *Rev. Sci. Instrum. Notes* **43**, No. 11, 1711-1712 (Nov. 1972).

Key words: Angular displacement detector; light emitting diode; phototransistors.

This Note describes a detector for small angular deflections (0.1  $\mu$ rad resolution). It uses a modulated infrared beam focused on a mirror whose angular deflection is to be measured. The beam is then reflected onto two phototransistors. The difference of the output voltages from these transistors is a measure of the angular displacement.

**13047.** Marzetta, L. A., **An evaluation of the three-voltmeter method for AC power measurement**, *IEEE Trans. Instr. Meas.* **IM-21**, No. 4, 353-357 (Nov. 1972).

Key words: Phase-sensitive detector; power-factor; quadrature; three-voltmeter method; wattmeter.

The accuracy and frequency response limitations in the present square-law responding laboratory wattmeters have promoted the search for alternate methods of ac power measurement using electronic instrumentation. The three-voltmeter method is based on an old principle of operation implemented by new analog circuitry. Results of the tests reported here show a precision of power calculation with 0.01 percent error at frequencies below 5 kHz. A unique test procedure is described for the comparison of the three-voltmeter device and a time-divisive multiplier wattmeter operating at zero power factor.

**13048.** Goodwin, R. D., **Thermophysical properties of methane**, *Proc. 2nd Conf. on Natural Gas Research and Technology*, Atlanta, Ga., June 5-7, 1972, Session V, Paper 2, pp. 1-12 (Institute of Gas Technology, Chicago, Ill., 1972).

Key words: Methane; pressure-density-temperature relations; thermodynamic properties.

This report describes briefly the rather direct methods recently used at this laboratory to prepare tables of provisional values of thermodynamic functions for methane. The basic data are spectroscopic specific heats for ideal gas states; the vapor pressure and melting curves; available virial coefficients for low density gas; and density (PVT) measurements over the domain from the triple point (90.68 K) to 400 K at pressures to 350 bar (1 atm = 1.01325 bar). References are given for the principal sources of PVT data.

The analytical descriptions of the PVT physical properties are emphasized in this report because they are needed for smoothing, for interpolation, and for the computation of derivatives. These have been developed here in recent years to be at least qualitatively consistent with known behavior about the critical point. The nonanalytic equation of state used here is qualitatively consistent with the experimental observation that specific heats  $C_p$  increase beyond measure upon close approach to the critical point.



**13049.** Goodwin, R. D., *Thermophysical properties of methane, Proc. 3rd Int. Conf. and Exhibition on Liquefied Natural Gas, Washington, D.C., Sept. 24-28, 1972, Session II, Paper 10*, pp. 1-12 (Institute of Gas Technology, Chicago, Ill., 1972).

**Key words:** Dielectric constants; methane, specific heats; thermal conductivities; thermodynamic functions; viscosities.

This report describes briefly the methods recently used at this laboratory to prepare tables of provisional values of thermodynamic functions for methane. References are given for the principal sources of PVT data. Emphasis is placed on analytical descriptions of physical properties because these are needed for smoothing, for interpolation, and for the computation of derivatives.

**13050.** Branscomb, L. M., *To help advance our Nation's scientific and technical capability for the greatest public benefit, Mater. Res. Stand. 12*, No. 5, 8-12 (May 1972).

**Key words:** Experimental incentive program; metrication; technology; standardization.

This interview presents an overview of the National Bureau of Standards in the context of its goal "to strengthen and advance the Nation's science and technology and to facilitate their effective application for public benefit."

**13051.** Kushner, L. M., *We have decided to become more active at the policy level in voluntary standardization activities, Mater. Res. Stand. 12*, No. 5, 13-14 (May 1972).

**Key words:** Engineering standards; standardization process; voluntary standardization.

The role of NBS in the voluntary standardization process used in this country is briefly outlined.

**13052.** Andrus, W. E., *A focus for the Bureau and all voluntary standardization organizations, Mater. Res. Stand. 12*, No. 5, 15-17 (May 1972).

**Key words:** Engineering standards; standardization; voluntary standards system.

In interview form, the role of the NBS program office for engineering and information processing standards is outlined. The voluntary product standards program is described, as are guidelines for NBS participation in standardizing bodies.

**13053.** Ambler, E., *A major innovation is our measurement assurance program, Mater. Res. Stand. 12*, No. 5, 18-23 (May 1972).

**Key words:** Basic standards; Josephson effect; lasers; metrology.

The mission and program of the NBS Institute for Basic Standards is presented in brief form. Calibration services, measurement assurance programs, and such new programs as laser stabilization and use of the Josephson junction in voltage monitoring are discussed.

**13054.** Hoffman, J. D., *IMR emphasizes accurate measurements and standards for materials, Mater. Res. Stand. 12*, No. 5, 24-33 (May 1972).

**Key words:** Air pollution measurements; failure analysis; materials research.

Such aspects of the NBS Institute for Materials Research as air pollution measurements, failure analysis, standard reference materials, high pressure research, surface research, collaborative research, and others are presented. The competences of the various IMR groups are tabulated, and problems, perspectives, and future opportunities are covered.

**13055.** Willenbrock, F. K., *We can never afford to be technically wrong, Mater. Res. Stand. 12*, No. 5, 34-36, 71-72 (May 1972)

**Key words:** Communications; consumer information; standardization.

A brief description of the NBS Institute for Materials Research is presented, especially as it impacts the public through information services and standardization activities.

**13056.** Young, T. R., *Laboratory evaluation: Facing up to a national problem, Mater. Res. Stand. 12*, No. 11, 22-26 (Nov. 1972).

**Key words:** Accreditation; certification; evaluation; national system; reference samples; testing laboratories.

A concept of a national system for evaluation and accreditation of testing laboratory functions is reviewed. Requesting laboratories having need would be provided examinations involving on-site inspections and reference sample audits supplied by national reference laboratories or task groups of individuals. The criteria used and the examiners would be recognized by a National Board who would also issue accreditations of testing functions having a public interest, based upon evaluation of laboratory examinations. Examples of existing reference laboratories are discussed.

**13057.** Rowland, G. A., *A program to assist the States in accepting industrialized housing, Mater. Res. Stand. 12*, No. 11, 17-21 (Nov. 1972).

**Key words:** Building codes; building manufacturer; Coordinated Evaluation System; engineering analysis; laboratory accreditation; Laboratory Evaluation and Accreditation Program (LEAP); Model Code Standardization Council; National Conference of States on Building Codes and Standards; quality assurance testing; testing laboratory.

The Laboratory Evaluation and Accreditation Program (LEAP) was established at the National Bureau of Standards to assist the States in the development of technical criteria and a methodology for the accreditation of institutions engaged in the evaluation of manufactured housing units for compliance with specified building codes. The needs of such a program were divided into: (1) a uniform national standard of reference; (2) a standard of laboratory competence; and (3) standards for uniform documentation of information. The program is concerned with: (1) engineering analysis; (2) physical testing; and (3) quality assurance.





## 5. INDEXES

### 5.1. HOW TO USE THE INDEXES

In addition to the usual author index, a subject index is provided in the form of a permuted key word index. In this type of index the key words in each publication or paper are arranged by shifting each group of key words along the horizontal printing line so that each key word in turn has an opportunity to appear alphabetically. The user is

thus able to locate papers of interest to him through the subject-related words he finds in the key word index.

The index symbols used in the author and key word indexes are explained in the following three tables. These tables also give the pages on which the abstracts of the various publication series begin.

Table A. Symbols for the Periodicals

NBS Journal of Research	Index Symbol			Issue Date	Page Number
	Vol.	Sec.	No.		
Section A	J76	A	1	January-February 1972	23
	J76	A	2	March-April 1972	24
	J76	A	3	May-June 1972	26
	J76	A	4	July-August 1972	27
	J76	A	5	September-October 1972	28
	J76	A	6	November-December 1972	30
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	J76	B	3 & 4	July-December 1972	33
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Table B. Symbols for the Nonperiodicals

NBS Nonperiodical Series	Index Symbol	Page Number
Monographs	Monogr.	38
Handbooks	H	40
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Table C. Symbols for the Papers Published By Others (1971)

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Laser induced damage; Light scattering; Stimulated Brillouin scattering; Bulk; Crystalline quartz; Fused quartz; Interaction gradient; Laser glass; *SP372*, pp. 11-14.

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Weights and measures inspection; Weights used by servicemen; Field standard weights; Specifications; Test weights; Tolerances; *H105-1. (Revised 1972)*.

Weights used by servicemen; Field standard weights; Specifications; Test weights; Tolerances; Weights and measures inspection; *H105-1. (Revised 1972)*.

Weiss model; Density of states; Ising model; Onsager model; Partition function; Phase transition; *SP323*, pp. 381-384.

Well crystal counting; Cadmium-109; Cobalt-57; Gamma-ray emission rate; Iron-57; Photoelectron escape; Silver-109m; Standardization; *12885*.

Wentzel theory; X-ray satellite lines; Auger transition; Coster-Kronig theory; Non-diagram lines; *12582*.

Wheel dressing; Abrasive wear parameter; Grinding; Material removal parameter; Principles of grinding; Surface finish in grinding; Surface integrity in ground surfaces; *SP348*, pp. 59-71.

Wheel machining; Abrasive; Ceramic machining; Sonic machining; Vibrational machining; *SP348*, pp. 133-139.

Wheel structure; Abrasive machining; Brittle chip formation; Brittle fracture; Chip accommodation; Glass; Glass-ceramics; Machining and grinding technical ceramics; Material removal rate; Specific energy; *SP348*, pp. 53-57.

Wide dynamic range; Fast integrator; High duty; Integral linearity; Stable converter; *12850*.

Wilmer Souder; Certification program; Guide; List of certified dental materials; Specifications; *12916*.

Wind; Coastal engineering; Damage; Hurricanes; Ocean waves; Probability theory; Storms; Storm surges; *12714*.

Wind loading; Window; Air-tightness; Performance characteristics; Performance parameters; Rain-tightness; Sealed glazing units; *SP361, Vol. 1*, pp. 375-384.

Wind vane; Work positioner; Conductometry; Decoding matrix; Fluoroolefins; Integrator; Magnetic sensing probe; Magnetic tape; Microbridge; Numbering machine; Perfluorostyrene; Shaft position encoder; Staple detector; Superconducting; *TN744*.

Window; Air-tightness; Performance characteristics; Performance parameters; Rain-tightness; Sealed glazing units; Wind loading; *SP361, Vol. 1*, pp. 375-384.

Window characteristics; Window evaluation; Window functions; Window requirements; Window standards; Performance criteria; Performance evaluation; *SP361, Vol. 1*, pp. 385-394.

Window evaluation; Window functions; Window requirements; Window standards; Performance criteria; Performance evaluation; Window characteristics; *SP361, Vol. 1*, pp. 385-394.

Window functions; Window requirements; Window standards; Performance criteria; Performance evaluation; Window characteristics; Window evaluation; *SP361, Vol. 1*, pp. 385-394.

Window materials; Actinometry; Experimental; Light sources; Photochemistry; Vacuum ultraviolet; *12942*.

Window materials; Infrared absorption; Infrared laser systems; Thermal fracture; *SP372*, pp. 172-175.

Window requirements; Window standards; Performance criteria; Performance evaluation; Window characteristics; Window evaluation; Window functions; *SP361, Vol. 1*, pp. 385-394.

Window standards; Performance criteria; Performance evaluation; Window characteristics; Window evaluation; Window functions; *SP361, Vol. 1*, pp. 385-394.

Winter masonry; Fresh mortar; Interaction between masonry mortars and units; Masonry mortar; Mortar evaluation; Mortar standard; Suction of masonry unit; *SP361, Vol. 1*, pp. 687-692.

Wire bond; Bonding; Degradation (wire bond); Discrete devices; Electrical interconnection; Fabrication (wire bond); Failure (wire bond); Hybrid circuits; Integrated circuits;



- Microelectronics; Reliability; Semiconductor devices; *TN726*.
- Wire bonding; Aluminum; Microelectronics; Ultrasonic bonding; *I3022*.
- Wire bonds; Alpha-particle detectors; Aluminum wire; Base transit time; Carrier lifetime; Die attachment; Electrical properties; Epitaxial silicon; Gamma-ray detectors; Germanium; Gold-doped silicon; Infrared response; Methods of measurement; *TN717*.
- Wire bonds; Alpha-particle detectors; Aluminum wire; Base transit time; Carrier lifetime; Die attachment; Electrical properties; Epitaxial silicon; Gamma-ray detectors; Germanium; Gold-doped silicon; Infrared response; Methods of measurement; *TN727*.
- Wire bonds; Aluminum wire; Base transit time; Carrier lifetime; Die attachment; Electrical properties; Epitaxial silicon; Gamma-ray detectors; Germanium; Gold-doped silicon; Infrared response; Methods of measurement; Microelectronics; Microwave diodes; *TN733*.
- Wire bonds; Aluminum wire; Base transit time; Carrier lifetime; Die attachment; Electrical properties; Epitaxial silicon; Gamma-ray detectors; Generation centers; Germanium; Gold-doped silicon; Infrared response; Methods of measurement; *TN743*.
- Wire samples; Elements; Fixed points; Reproducibility; Superconductors; Thermometry; Transition widths; *I2511*.
- Wire-bond; Bibliography; Degradation (wire-bond); Discrete devices; Electrical interconnection; Fabrication (wire-bond); Failure (wire-bond); Hybrid circuits; Integrated circuits; Microelectronics; Reliability; Testing (wire-bond); *TN593*.
- Wood frame; Building; Design criteria; Drift; Field test; Floor vibration; *SP361, Vol. 1*, pp. 275-288.
- Word lengths as block codes; Speech intelligibility as channel capacity; Articulation function of ear; "bit" capacity of ear; Channel capacity of ear; Distinctive features of ear and hearing; Intelligibility vs word lengths as block codes; Speech; *I2442*.
- Word-term pairing; Automatic indexing; COBOL; Document records; Programming; Statistical analysis; Teaching sample; *I2858*.
- Work function; Adsorption; Field emission; Methane; Physical adsorption; Single crystal; Tungsten; *I2735*.
- Work function; Binding energy; Chemisorption; Displacement; Hydrogen; Methane; Oxygen; Tungsten; *I2736*.
- Work function; Carbon contamination; Electronic density of states; Photoemission; Tungsten (W); UV photoemission; *SP323*, pp. 199-203.
- Work hardening; Equivalent strain; Hardening; Plasticity; Strain hardening; *J.76C Nos. 1 and 2*, 53-54 (1972).
- Work positioner; Conductometry; Decoding matrix; Fluoroolefins; Integrator; Magnetic sensing probe; Magnetic tape; Microbridge; Numbering machine; Perfluorostyrene; Shaft position encoder; Staple detector; Superconducting; Synthesis, chemical; *TN744*.
- World trade; Cryogenics; Economic forecasts; International conferences; Liquefied natural gas; *I2616*.
- W-Re; Alloys; Bcc transition metal alloys; Charging effect; Electronic density of states; Ginzburg-Landau coherence length; G.P. zone; Hf-Ta; Low-temperature specific heat; Magnetic susceptibility; Omega phase; *SP323*, pp. 587-596.
- WWV; High frequency; Standard radio frequencies; Time-frequency broadcasts; Time signals; *TN611*.
- WWV; WWVH; Clocks; H. F. Broadcasts; Sunspot cycle; Time signals; *I2594*.
- WWVH; Clocks; H. F. Broadcasts; Sunspot cycle; Time signals; WWV; *I2594*.
- X ray; Alloys; Dislocation; Stacking-fault energy; Stacking-fault probability; *I2893*.
- X ray; Bromine; Copper; Crystal; Pyridine *N*-oxide; Structure; *I2661*.
- X ray; Cadmium; Coordination complex; Crystal structure; Imidazole; *I2546*.
- X ray; Law enforcement; Voluntary standards; *I2781*.
- X rays; Attention coefficient; Compilation; Compton scattering; Photo electric effect; Photons; *I2648*.
- X rays; Attenuation coefficient; Bibliography; Cross section; Data index; Gamma rays; Photons; *I2800*.
- X rays; Depth-dose dyes; Dose distribution; Dosimetry; Electrons; Films; Gamma rays; Gels; Radiation beams; *I2455*.
- X rays; Diffraction; Fluorescence analysis; Radiation safety; *I2484*.
- Xenon; Autoionization; Far ultraviolet; Krypton; Photoionization; Resonances; *J.76A No. 1, 1-12* (1972).
- Xenon; Autoionization; Far ultraviolet; Krypton; Photoionization; Resonances; *I2691*.
- Xenon; Compressibility; Critical point; Equation of state; Fluid; Helium; Low temperature; Methane; Scaling law; Specific heat; *J.76A No. 3*, 207-211 (1972).
- Xenon; Electronic density of states; Electron synchrotron light; Krypton; Optical absorption; *SP323*, p. 279.
- X-ray absorption; X-ray emission; Electron probe microanalysis; Errors; Fluorescence; Iteration; *I2537*.
- X-ray absorption; X-ray inelastic scattering; Compton scattering; Plasmon scattering; Raman scattering; Relation between spectra; *I2409*.
- X-ray analysis; Absorption; Atomic number; Chemical elements; Computation procedure; Data reduction; Electron probe microanalysis; Fluorescence; Time-sharing; *TN719*.
- X-ray crystal structure; Bismuth; Borate; *I2903*.
- X-ray diffraction; Amorphous boron; Anhydrous boric acid; Boric oxide; Boron carbide structure type; Boron suboxide; Crystal structure; Decompose; Electron microbeam probe; Infrared spectrum; Lattice parameters; Pycnometer; *SP364*, pp. 605-611.
- X-ray diffraction; Austenite; Computer; Ferrite; Phase measurement; Quantitative analysis; Retained austenite; *TN709*.
- X-ray diffraction; Calcium coordinations; Calcium phosphates; Hydrogen bonding; Monetite single crystals; *I2914*.
- X-ray diffraction; Crystal structure; Integrated intensities; Lattice constants; Peak intensities; Powder patterns; Reference intensities; Standard; *Monogr. 25, Section 10*.
- X-ray diffraction; Density expansion; Liquid structure factor; Liquid theory; Neutron diffraction; Pair correlation function; *I2795*.
- X-ray diffraction; X-ray fluorescence; Applied x-ray analysis; Conference report; Material analysis; *I2472*.
- X-ray diffraction data; Binary halides; Crystal structure transformation; Electronic data; Phase transformation; Spectroscopic data; Thermodynamic data; *NSRDS-NBS41*.
- X-ray emission; Electron bombardment; Lead myristate analyzing crystal; M. O. correlation; Nitrogen *K* emission spectrum; Resonance radiation; *I2738*.
- X-ray emission; Electron probe microanalysis; Errors; Fluorescence; Iteration; X-ray absorption; *I2537*.
- X-ray emission; Electronic density of states; Ferromagnetism; Iron; Optical reflection; Photoemission; *SP323*, pp. 47-52.
- X-ray emission and absorption; Density of states; Interacting electrons; One-particle Green function; Oscillator strengths; Quasi particle density of states; *SP323*, pp. 233-247.
- X-ray equipment; Radiation safety; *H111*.
- X-ray fluorescence; Applied x-ray analysis; Conference report; Material analysis; X-ray diffraction; *I2472*.
- X-ray fluorescence analysis; Analysis; Computer program; Electron probe; Microanalysis; Optical spectrometry; Pre-concentration techniques; Spectrochemical analysis; Standard reference materials; *TN582*.
- X-ray inelastic scattering; Collective excitations; Energy transfer; Lithium; Momentum transfer; *I2575*.

X-ray inelastic scattering; Compton scattering; Plasmon scattering; Raman scattering; Relation between spectra; X-ray absorption; 12409.

X-ray investigations; Binary system; Boron; Carbon; Chemical analysis; Melting-point determination; Metallography; Phase-field division; Silicon; Solubilities; Ternary system; *SP364*, pp. 505-513.

X-ray  $L_{23}$  emission; Argon; Configuration interaction; KCl; Radiative process; Two electron processes; 12692.

X-ray photoelectron spectroscopy; Electronic density of states; Gold aluminum two ( $\text{AuAl}_2$ ); Gold gallium two ( $\text{AuGa}_2$ ); *SP323*, pp. 791-793.

X-ray photoemission; Aluminum; Auger-peak; Secondary-electron energy distribution; 12720.

X-ray photoemission; Aluminum; Electronic density of states; Photoelectron energy distribution; 12964.

X-ray photoemission; Barium (Ba);  $\beta$ -tungsten compounds; Effects of oxidation; Electronic density of states; Europium (Eu); Lanthanides; Matrix elements; Photoemission; Rare-earth metals; UV and x-ray photoemission; *SP323*, pp. 217-220.

X-ray photoemission;  $\text{ZnS}$ ;  $\text{CdCl}_2$ ; Density of states;  $\text{HgO}$ ; Noble metals; Rigid band model; Transition metals; *SP323*, pp. 163-178.

X-ray photoemission spectroscopy; Alloys; Aluminum; Gallium; Gold; Indium; Intermetallic compound; Knight shift; Relaxation time; Soft x-ray spectroscopy; 12721.

X-ray Raman effect; Absorption; Charge correlation; Compton effect; Core electrons; Current correlation; Inelastic scattering; Solid; Theory; Valence electrons; 12542.

X-ray satellite lines; Auger transition; Coster-Kronig theory; Non-diagram lines; Wentzel theory; 12582.

X-ray spectroscopy; Zinc (Zn); Cobalt; Copper; Electronic density of states; Iron; Nickel; Satellite emissions; Self absorption; Soft x-ray emission; *SP323*, pp. 319-326.

X-ray structure determination; Alkali metal; Bronze; Heptagonal holes; Hexagonal tungsten bronze; Lattice image; Molybdate; Molybdenum; Niobate; Niobium; Oxide; Single crystal; Tetramolybdate; *SP364*, pp. 15-27.

X-ray-diffraction crystallography; Crystallography; Crystal structure/alloys; Gold-cadmium alloys; Phase transformations/solid state; 13036.

X-rays; Attenuation coefficient; Coherent scattering; Compilation; Cross section; Incoherent scattering; Photoelectric absorption; Photons; 12868.

$X^2\Pi$ ;  $A^2\Sigma$ ; Electronic transition probabilities; Hartree-Fock;  $\text{LiO}$ ; Vibrational transition probabilities; *J.76A No. 6*, 665-668 (1972).

## Y

Yellowing; Atmospheric pollutants; Color—difference and representation; Impact resistance; Plastics; Rigid polyvinyl chloride (PVC); Test methods; Ultraviolet (UV) radiation; Water vapor; Weathering—artificial and natural; *SP361, Vol. 1*, pp. 751-760.

Yielding; Anisotropy; Continuum mechanics; Entaxy; Entropy; Irreversibility; Non-equilibrium state; Nonlinear theory; Plasticity; Thermodynamics; Viscoelasticity; 12948.

Youden's burette experiment; Accuracy; Analysis of variance; Measurement process; Precision; Regression line; Scheduling measurements; Statistical design of experiments; Systematic error; 12527.

Young's modulus; Cold-work; Dislocation relaxation; Internal friction;  $n$ -alkane; Relaxation process; 12581.

Yttrium; Spectra; Ultraviolet; Wavelengths; 12826.

Yttrium; Zirconium; Molybdenum; Niobium; Rubidium; Spectra; Strontium; Ultraviolet; Wavelengths; 12675.

## Z

Z average molecular weight; Density; Differential refractive index; Gel permeation chromatography (GPC); Light scattering; Linear polyethylene; Melt flow rate; Molecular weight distribution; Number average molecular weight; Osmometry; Refractive index; *SP260-42*.

Zeros of polynomials in regular sets; Basic sets; Cannon sum of basic sets; Lower semiblock matrices; Order of basic sets; *J.76B Nos. 3 and 4*, 153-159 (1972).

Zinc; Aluminum; Cadmium; Cryogenics; Indium; Lead; Magnetic susceptibility; Superconductive transition temperature; Superconductivity; Thermometric fixed points; *SP260-44*.

Zinc nuclei; Electron scattering; Nuclear radii; Nuclear sizes; 12928.

Zinc oxide-EBA-eugenol cements; Crown and bridge cements; Dental cements; EBA cements; EBA sedative bases; Intermediate restorative; *o*-ethoxybenzoic acid cements; Pulp capping materials; *SP354*, pp. 101-111.

Zinc (Zn); Cobalt; Copper; Electronic density of states; Iron; Nickel; Satellite emissions; Self absorption; Soft x-ray emission; X-ray spectroscopy; *SP323*, pp. 319-326.

Zinc (Zn); Dielectric constant; Electronic density of states; Molybdenum (Mo); Optical density of states; Optical properties; Photoemission; Reflectivity; Tungsten (W); *SP323*, pp. 209-215.

Zincblende;  $\text{ZnSe}$ ; Aluminum phosphide (AlP); Electronic density of states; Exchange potential; Gallium arsenide (GaAs); Germanium; Self-consistent orthogonalized plane wave model (SCOPW); Semiconductors, tetrahedrally bonded; Silicon; *SP323*, pp. 93-102.

Zincblende structure;  $\text{ZnTe}$ ; Electronic density of states; Gallium arsenide (GaAs); Indium antimony (InSb); Indium arsenide (InAs); Joint density of states; Nonlinear optical susceptibility; Optical properties; *SP323*, pp. 757-766.

Zirconium; Anderson Hamiltonian; Barium (Ba); Calcium; Chemisorption; Electron density of states; Field-emission resonance tunneling; Germanium; Tungsten (W); Tunneling; *SP323*, pp. 375-379.

Zirconium (Zr); Copper; Direct versus nondirect transitions; Electronic density of states; Gold (Au); Nondirect transitions; Optical density-of-states; Photoemission; Scandium (Sc); Silver (Ag); Titanium (Ti); *SP323*, pp. 205-208.

Zirconium-niobium oxide; Crystal structure; Intergrrowth; Lattice-image; Polymorphism; *SP364*, pp. 165-182.

$\text{ZnS}$ ;  $\text{CdCl}_2$ ; Density of states;  $\text{HgO}$ ; Noble metals; Rigid band model; Transition metals; X-ray photoemission; *SP323*, pp. 163-178.

$\text{ZnS}$ ;  $\text{Zn}_x\text{Cd}_{1-x}\text{S}$ ; Laser Raman spectra; Polycrystalline; *SP364*, p. 721.

$\text{ZnSe}$ ; Aluminum phosphide (AlP); Electronic density of states; Exchange potential; Gallium arsenide (GaAs); Germanium; Self-consistent orthogonalized plane wave model (SCOPW); Semiconductors, tetrahedrally bonded; Silicon; Zincblende; *SP323*, pp. 93-102.

$\text{ZnTe}$ ; Electronic density of states; Gallium arsenide (GaAs); Indium antimony (InSb); Indium arsenide (InAs); Joint density of states; Nonlinear optical susceptibility; Optical properties; Semiconductors; *SP323*, pp. 757-766.

$\text{Zn}_x\text{Cd}_{1-x}\text{S}$ ; Laser Raman spectra; Polycrystalline;  $\text{ZnS}$ ; *SP364*, p. 721.

Zonal harmonics; Diurnal phase; Omega; Time; Time dissemination; VLF propagation; *TN610*.

1 N  $\text{H}_2\text{SO}_4$ ; Oxide; Passive; Spinel; Amorphous; Diffraction; Fe-Cr; Lattice parameter; 13004.

1-butene; 2-butene; Concurrent reactions; Consecutive reactions; Controlled oxidation; Conventional additive experiments; Cool-flames; Intermediate products; Isobutane; Isotopic tracer techniques; Isotopically-labelled additives; *SP357*, pp. 111-117.



- 1-chloronaphthalene; 1,2,4-trichlorobenzene; Decalin; Limiting viscosity number; Linear polyethylene; Solution viscosity; Viscometer; *J.76A No. 2, 147-149 (1972)*.
- 1-chloronaphthalene; 1,2,4-trichlorobenzene; Differential refractive index;  $dn/dc$ ; Refractive index; Refractometer; *J.76A No. 2, 151-155 (1972)*.
- $^{12}\text{C}$ ,  $^{13}\text{C}$ ; Continuum spectra; Efficiencies; Fine structure; Giant resonance; Isospin splitting; Pygmy; Pygmy resonance; Radiative tails; Resonance weak coupling; *12929*.
- $^{121}\text{Sb}$ ; Alloys; Hyperfine fields; Mössbauer effect; Order-disorder; *12865*.
- 1,2,4-trichlorobenzene; Decalin; Limiting viscosity number; Linear polyethylene; Solution viscosity; Viscometer; 1-chloronaphthalene; *J.76A No. 2, 147-149 (1972)*.
- 1,2,4-trichlorobenzene; Differential refractive index;  $dn/dc$ ; Refractive index; Refractometer; 1-chloronaphthalene; *J.76A No. 2, 151-155 (1972)*.
- $^{13}\text{C}$  n.m.r. spectroscopy;  $^{19}\text{F}$  n.m.r. spectroscopy; Internuclear double resonance; Internuclear triple resonance; Nitrogen-15 coupling constants; Nuclear Overhauser effects; P.m.r. spectroscopy; *12444*.
- $^{13}\text{C}$  relaxation; Chemical shift anisotropy; Dipole-dipole; Scalar relaxation; Spin-rotation;  $T_1$ ;  $T_2$ ; *12592*.
- 1,4-dioxane; Kinetics; Mechanism; Organic compound; Oxidative degradation; Peroxy radical isomerization; Poly(ethylene oxide); Polymer; Polypropylene; Poly(propylene oxide); Polystyrene; Polytetrahydrofuran; Room temperature; *SP357*, pp. 85-92.
- 15 MeV electrons;  $^{60}\text{Co}$  gamma rays; Absorbed dose;  $\text{CaF}_2$ ; Dy; Dosimeters; LiF; Response; Thermoluminescence; *12833*.
- $^{15}\text{N}$ -labeled amino sugars; Infrared isotopic shift; Mass spectrometry; Nucleophilic substitution;  $^{15}\text{N}$ -trifluoroacetyl derivative; Derivatives of 6-amino-6-deoxy-D-glucose-6- $^{15}\text{N}$ ; Differential scanning calorimetry; *12443*.
- $^{15}\text{N}$ -trifluoroacetyl derivative; Derivatives of 6-amino-6-deoxy-D-glucose-6- $^{15}\text{N}$ ; Differential scanning calorimetry;  $^{15}\text{N}$ -labeled amino sugars; Infrared isotopic shift; Mass spectrometry; Nucleophilic substitution; *12443*.
- $^{19}\text{F}$  n.m.r. spectroscopy; Internuclear double resonance; Internuclear triple resonance; Nitrogen-15 coupling constants; Nuclear Overhauser effects; P.m.r. spectroscopy; 6-amino-6-deoxy-D-glucose-6- $^{15}\text{N}$  derivatives; *12444*.
- 2-butene; Concurrent reactions; Consecutive reactions; Controlled oxidation; Conventional additive experiments; Cool-flames; Intermediate products; Isobutane; Isotopic tracer techniques; Isotopically-labelled additives; Macroscopic stages; *SP357*, pp. 111-117.
- 2-generator groups; parabolic classes; Fuchsian groups; *12704*.
- $^{20}\text{Ne}$ ;  $^{22}\text{Ne}$ ; Boiling point; Neon; Neon isotopes; Neon point; Triple point; Vapor pressure; *12597*.
- $^{22}\text{Ne}$ ; Boiling point; Neon; Neon isotopes; Neon point; Triple point; Vapor pressure;  $^{20}\text{Ne}$ ; *12597*.
- 2,2,3-trimethylbutane; Bond energy; Cyclohexane; Decomposition; Gas phase; Isopropyl bromide; Shock tube; *t*-butyl radical decyclization; *12831*.
- 2,2,3-trimethylpentane; Bond energy; Cyclohexyl radical; 3,4-dimethylhexane; Heats of formation; *n*-propyl radical; *s*-butyl radical; Shock tube; *t*-butyl radical; Thermal decomposition; *12562*.
- 2,3,3,3-tetrafluoropropene; Polymerization; Pressure; Radiation-induced; Tetrafluoroethylene; *12384*.
- $^{252}\text{Cf}$ ; Manganous sulfate bath; Neutron emission rate; Neutron sources; Neutron spectra; Neutron spectrum measurement methods; *12880*.
- 3d edges; Erbium; Photoabsorption; Theory; Thulium; *13045*.
- $^3\text{He}(pd)$  vertex; Plane wave impulse approximations; Quasi-free scattering; Separable potentials; Three-body problem; Confidence cross sections; *13012*.
- 3-13 GeV electron beam; Photon energy; Production cross sections; Spallation products; *12856*.
- 3.39  $\mu\text{m}$  laser;  $\text{CO}_2$  laser; Helium neon laser; Laser frequency measurement; MOM diode; *12529*.
- 3,4-dimethylhexane; Heats of formation; *n*-propyl radical; *s*-butyl radical; Shock tube; *t*-butyl radical; Thermal decomposition; 2,2,3-trimethylpentane; Bond energy; Cyclohexyl radical; *12562*.
- $35 \times 70$ ; Coupling coefficients; Permutation symmetry; Quark interchange; Relative phases,  $SU(6)$  multiplets; *12639*.
- 4  $f^\pi$  configurations; Complex ions; Coordination polyhedra; Nonstoichiometry; Polymolecular frameworks; Rare earth optical spectra; Rare earth oxide; Refractory materials; Thin films; *SP364*, pp. 367-383.
- $^4\text{He}$  photodisintegration; E-2 angular distributions; Electric quadrupole transition; Identical particles; Virtual photons; *12878*.
- 4-methylpentyne-1; Allene; Bond energy; Comparative rate; Gas phase; Heats of formation; Kinetics; Molecular reaction; Propynyl; Pyrolysis; Single pulse shock tube; *12832*.
- 6-amino-6-deoxy-D-glucose-6- $^{15}\text{N}$  derivatives;  $^{13}\text{C}$  n.m.r. spectroscopy;  $^{19}\text{F}$  n.m.r. spectroscopy; Internuclear double resonance; Internuclear triple resonance; Nitrogen-15 coupling constants; Nuclear Overhauser effects; *12444*.
- 6-deoxy- $\alpha$ -D-glucopyranose derivative; General Overhauser effect; Internuclear double resonance; Long-range coupling; Magnetic equivalence factoring; Spin-tickling; Transient nutations; *12693*.
- 60-Hz power line; Atomic clock; Frequency calibration; Frequency stability; Optical pulsars; Remote clock comparisons; Simultaneous reception; Time dissemination; Time stability; Time synchronization; Time transfer; TV color subcarrier; *12986*.
- $^{82}\text{Br}$ ; Beta rays; Gamma rays; Hyperfine interactions; Isotope separator; Magnetic moment; Nuclear orientation; *12888*.





# APPENDIX A. LIST OF DEPOSITORY LIBRARIES IN THE UNITED STATES

## ALABAMA

Alexander City: Alexander City State Junior College, Thomas D. Russell Library (1967).  
 Auburn: Auburn University, Ralph Brown Draughon Library (1907).  
 Birmingham:  
   Birmingham Public Library (1895).  
   Birmingham-Southern College Library (1932).  
   Jefferson State Junior College, James B. Allen Library (1970).  
   Samford University, Harwell G. Davis Library (1884).  
 Enterprise: Enterprise State Junior College Library (1967).  
 Florence: Florence State University, Collier Library (1932).  
 Gadsden: Gadsden Public Library (1963).  
 Huntsville: University of Alabama, Huntsville Campus Library (1964).  
 Jacksonville: Jacksonville State University, Romana Wood Library (1929).  
 Maxwell A.F. Base: Air University Library (1963).  
 Mobile:  
   Mobile Public Library (1963).  
   Spring Hill College, Thomas Byrne Memorial Library (1937).  
   University of South Alabama Library (1968).  
 Montgomery:  
   Alabama State Department of Archives and History Library (1884).  
   Alabama Supreme Court Library (1884).  
   Auburn University at Montgomery Library (1971).  
 Normal: Alabama Agricultural and Mechanical College, Drake Memorial Library (1963).  
 St. Bernard: St. Bernard College Library (1962).  
 Troy: Troy State University, Lurleen B. Wallace Educational Resources Center (1963).  
 Tuskegee Institute: Tuskegee Institute, Hollis Burke Frissell Library (1907).  
 University:  
   University of Alabama School of Law Library (1967).  
   University of Alabama Library (1860) – REGIONAL

## ALASKA

Anchorage:  
   Anchorage Community College Library (1961).  
   Anchorage Methodist University Library (1963).  
 College: University of Alaska, Elmer E. Rasmuson Library (1922).  
 Juneau: Alaska State Library (1964).  
 Ketchikan: Ketchikan Community College Library (1970).

## ARIZONA

Flagstaff: Northern Arizona University Library (1937).  
 Phoenix:  
   Department of Library and Archives (unknown) – REGIONAL.  
   Phoenix Public Library (1917).

Prescott: Prescott College Library (1968).  
 Tempe: Arizona State University, Matthews Library (1944).  
 Thatcher: Eastern Arizona College Library (1963).  
 Tucson:  
   Tucson Public Library (1970).  
   University of Arizona Library (1907) – REGIONAL.  
 Yuma: Yuma City-County Library (1963).

## ARKANSAS

Arkadelphia: Quachita Baptist University, Riley Library (1963).  
 Batesville: Arkansas College Library (1963).  
 Clarksville: College of the Ozarks Library (1925).  
 Conway: Hendrix College, O. C. Bailey Library (1903).  
 Fayetteville: University of Arkansas Library (1907).  
 Little Rock:  
   Arkansas Supreme Court Library (1962).  
   Little Rock Public Library (1953).  
 Magnolia: Southern State College, J. M. Peace Library (1956).  
 Monticello: University of Arkansas at Monticello Library (1956).  
 Russellville: Arkansas Polytechnic College, Tomlinson Library (1925).  
 Searcy: Harding College, Beaumont Memorial Library (1963).  
 State College: Arkansas State University, Dean B. Ellis Library (1913).  
 Walnut Ridge: Southern Baptist College, Felix Goodson Library (1967).

## CALIFORNIA

Anaheim: Anaheim Public Library (1963).  
 Arcata: Humboldt State College Library (1963).  
 Bakersfield: Kern County Library (1943).  
 Berkeley:  
   University of California, General Library (1907).  
   University of California, Law Library, Earl Warren Legal Center (1963).  
 Chico: Chico State University Library (1962).  
 Claremont: Pomona College Documents Collection, Honnold Library (1913).  
 Compton: Compton Library (1972).  
 Culver City: Culver City Library (1966).  
 Davis:  
   University of California at Davis Library (1953).  
   University of California at Davis, School of Law Library (1972).  
 Downey: Downey City Library (1963).  
 Fresno:  
   Fresno County Free Library (1920).  
   California State University Library (1962).  
 Fullerton: California State College at Fullerton Library (1963).  
 Garden Grove: Adult Reference Center Library (1963).  
 Gardena: Gardena Public Library (1966).  
 Hayward: California State College at Hayward Library (1963).  
 Huntington Park: Huntington Park Library, San Antonio Region (1970).  
 Inglewood: Inglewood Public Library (1963).

Irvine: University of California at Irvine Library (1963).  
 La Jolla: University of California, San Diego, University Library (1963).  
 Lakewood: Angelo Jacoboni Public Library (1970).  
 Lancaster: Lancaster Regional Library (1967).  
 Long Beach:  
   California State College at Long Beach Library (1962).  
   Long Beach Public Library (1933).  
 Los Angeles:  
   California State College at Los Angeles, John F. Kennedy Memorial Library (1956).  
   Los Angeles County Law Library (1963).  
   Los Angeles Public Library (1891).  
   Loyola University of Los Angeles Library (1933).  
   Occidental College, Mary Norton Clapp Library (1941).  
   Pepperdine University Library (1963).  
   University of California at Los Angeles Library (1932).  
   University of California at Los Angeles, Law Library (1958).  
   University of Southern California Library (1933).  
 Menlo Park: Department of the Interior, Geological Survey Library (1962).  
 Montebello: Montebello Library (1966).  
 Monterey: Naval Postgraduate School Library (1963).  
 Monterey Park: Bruggemeyer Memorial Library (1964).  
 Northridge: San Fernando Valley State College Library (1958).  
 Oakland:  
   Mills College Library (1966).  
   Oakland Public Library (1923).  
 Pasadena:  
   California Institute of Technology, Millikan Memorial Library (1933).  
   Pasadena Public Library (1963).  
 Pleasant Hill: Contra Costa County Library (1964).  
 Redding: Shasta County Library (1956).  
 Redlands: University of Redlands, Armacost Library (1933).  
 Redwood City: Redwood City Public Library (1966).  
 Reseda: West Valley Regional Branch Library (1966).  
 Richmond: Richmond Public Library (1943).  
 Riverside:  
   Riverside Public Library (1947).  
   University of California at Riverside Library (1963).  
 Sacramento:  
   California State Library (1895) – REGIONAL.  
   Sacramento City-County Library (1880).  
   Sacramento County Law Library (1963).  
   Sacramento State College Library (1963).  
 San Bernardino: San Bernardino County Free Library (1964).  
 San Diego:  
   San Diego County Library (1966).  
   San Diego Public Library (1895).  
   San Diego State College, Love Library (1962).  
   University of San Diego Law Library (1967).  
 San Francisco:  
   Mechanics' Institute Library (1889).  
   San Francisco Public Library (1889).  
   San Francisco State College, Social Science and Business Library (1955).  
   U.S. Court of Appeals for Ninth Circuit Library (1971).  
   University of San Francisco, Richard A. Gleeson Library (1963).  
 San Jose: San Jose State College Library (1962).  
 San Leandro: San Leandro Community Library Center (1961).  
 San Luis Obispo: California State Polytechnic University Library (1969).  
 Santa Ana: Santa Ana Public Library (1959).  
 Santa Barbara: University of California at Santa Barbara Library (1960).

Santa Clara: University of Santa Clara, Orradre Library (1963).  
 Santa Cruz: University of California at Santa Cruz Library (1963).  
 Santa Rosa: Santa Rosa-Sonoma County Public Library (1896).  
 Stanford: Stanford University Libraries (1895).  
 Stockton: Public Library of Stockton and San Joaquin County (1884).  
 Thousand Oaks: California Lutheran College Library (1964).  
 Torrance: Torrance Civic Center Library (1969).  
 Turlock: Stanislaus State College Library (1964).  
 Valencia: Valencia Regional Library (1972).  
 Van Nuys: Los Angeles Valley College Library (1970).  
 Visalia: Tulare County Free Library (1967).  
 Walnut: Mount San Antonio College Library (1966).  
 West Covina: West Covina Library (1966).  
 Whittier: Whittier College, Wardman Library (1963).

## CANAL ZONE

Balboa Heights: Canal Zone Library-Museum (1963).

## COLORADO

Alamosa: Adams State College Learning Resources Center (1963).  
 Boulder: University of Colorado Libraries (1879) – REGIONAL.  
 Colorado Springs: Colorado College, Charles Leaming Tutt Library (1880).  
 Denver:  
   Colorado State Library (unknown).  
   Denver Public Library (1884) – REGIONAL.  
   Department of Interior, Bureau of Reclamation Library (1962).  
   Regis College, Dayton Memorial Library (1915).  
   University of Denver, Mary Reed Library (1909).  
 Fort Collins: Colorado State University Library (1907).  
 Golden:  
   Colorado School of Mines, Arthur Lakes Library (1939).  
   Jefferson County Public Library, Bonfils-Stanton Regional Library (1968).  
 Greeley: University of Northern Colorado Library (1966).  
 Gunnison: Western State College, Leslie J. Savage Library (1932).  
 La Junta: Otero Junior College, Wheeler Library (1963).  
 Pueblo:  
   Pueblo Regional Library (1893).  
   Southern Colorado State College Library (1965).  
 U.S. Air Force Academy: Academy Library (1956).

## CONNECTICUT

Bridgeport: Bridgeport Public Library (1884).  
 Danbury: Western Connecticut State College, Ruth A. Haas Library (1967).  
 Enfield: Enfield Public Library (1967).  
 Hartford:  
   Connecticut State Library (unknown) – REGIONAL.  
   Hartford Public Library (1945).  
   Trinity College Library (1895).  
 Middletown: Wesleyan University Library (1906).  
 Mystic: Marine Historical Association, Inc., Mystic Seaport Library (1964).  
 New Haven:  
   Southern Connecticut State College Library (1968).  
   Yale University Library (1859).



New London:

Connecticut College Library (1926).

U.S. Coast Guard Academy Library (1939).

Pomfret: Pomfret School Library (1968).

Storrs: University of Connecticut, Wilbur Cross Library (1907).

Waterbury: Silas Bronson Library (1869).

West Haven: University of New Haven Library (1971).

## DELAWARE

Dover:

Delaware State College, William C. Jason Library (1962).

State Law Library in Kent County (unknown).

Georgetown: Delaware Technical and Community College, Southern Branch Library (1968).

Newark: University of Delaware, Morris Library (1907).

Wilmington: Wilmington Institute and New Castle County Library (1861).

## DISTRICT OF COLUMBIA

Washington:

Advisory Commission on Intergovernmental Relations Library.

Civil Service Commission Library (1963).

Department of Commerce Library (1955).

Department of Health, Education, and Welfare Library (1954).

Department of Housing and Urban Development Library (1969).

Department of the Interior Central Library (1895).

Department of the Interior, Geological Survey Library (1962).

Department of Justice Main Library (1895).

Department of State Library (1895).

Department of State, Office of Legal Advisor, Law Library (1966).

Department of Transportation, National Highway Traffic Safety Administration Library (1968).

District of Columbia Public Library (1943).

Federal Bureau of Investigation Academy Library (1970).

Federal City College Library (1970).

Federal Deposit Insurance Corporation Library (1972).

Georgetown University Library (1969).

Indian Claims Commission Library (1968).

National Agricultural Library (1895).

National War College Library (1895).

Navy Department Library (1895).

Navy Department, Office of Judge Advocate General Library (1963).

Office of Management and Budget Library (1965).

Office of the Adjutant General, Department of Army Library (1969).

Postal Service Library (1895).

Treasury Department Library (1895).

Veterans Administration, Central Office Library (1967).

## FLORIDA

Boca Raton: Florida Atlantic University Library (1963).

Clearwater: Clearwater Public Library (1972).

Coral Gables: University of Miami Library (1939).

Daytona Beach: Volusia County Public Libraries (1963).

De Land: Stetson University, duPont-Ball Library (1887).

Fort Lauderdale:

Fort Lauderdale Public Library (1967).

Nova University Library (1967).

Gainesville: University of Florida Libraries (1907)—REGIONAL.

Jacksonville:

Haydon Burns Library (1914).

Jacksonville University, Swisher Library (1962).

University of North Florida Library (1972).

Lakeland: Lakeland Public Library (1928).

Leesburg: Lake-Sumter Community College Library (1963).

Melbourne: Florida Institute of Technology Library (1963).

Miami:

Florida International University Library (1970).

Miami-Dade Junior College, North Campus Library (1967).

Miami Public Library (1952).

Opa Locka: Biscayne College Library (1966).

Orlando: Florida Technological University Library (1966).

Palatka: St. Johns River Junior College Library (1963).

Pensacola: University of West Florida, John C. Pace Library (1966).

St. Petersburg: St. Petersburg Public Library (1965).

Sarasota: Sarasota Public Library (1970).

Tallahassee:

Florida Agricultural and Mechanical University, Coleman Memorial Library (1936).

Florida State Library (1929).

Florida State University, R. M. Strozier Library (1941).

Tampa:

Tampa Public Library (1965).

University of South Florida Library (1962).

University of Tampa, Merle Kelce Library (1953).

Winter Park: Rollins College, Mills Memorial Library (1909).

## GEORGIA

Albany: Albany Public Library (1964).

Americus: Georgia Southwestern College, Wade Lott Memorial Library (1966).

Athens: University of Georgia Libraries (1907).

Atlanta:

Atlanta Public Library (1880).

Atlanta University, Trevor Arnett Library (1962).

Emory University, Robert W. Woodruff Library (1928).

Emory University, School of Law Library (1968).

Georgia Institute of Technology, Prince Gilbert Memorial Library (1963).

Georgia State Library (unknown).

Georgia State University Library (1970).

Augusta: Augusta College Library (1962).

Brunswick: Brunswick Public Library (1965).

Carrollton: West Georgia College, Sanford Library (1962).

Dahlonega: North Georgia College Library (1939).

Gainesville: Chestatee Regional Library (1968).

Macon: Mercer University Library (1964).

Marietta: Kennesaw Junior College Library (1968).

Milledgeville: Georgia College at Milledgeville, Ina Dillard Russell Library (1950).

Mount Berry: Berry College, Memorial Library (1970).

Savannah: Savannah Public and Chatham-Effingham Liberty Regional Library (1857).

Statesboro: Georgia Southern College, Rosenwald Library (1939).

Valdosta: Valdosta State College, Richard Holmes Powell Library (1956).

## GUAM

Agana: Nieves M. Flores Memorial Library (1962).

## HAWAII

Hilo: University of Hawaii, Hilo Campus Library (1962).  
Honolulu:  
Chaminade College of Honolulu Library (1965).  
Hawaii Medical Library, Inc. (1968).  
Hawaii State Library (1929).  
Municipal Reference Library of the City and County of Honolulu (1965).  
University of Hawaii Library (1907).  
Laie: Church College of Hawaii Library (1964).  
Lihue: Kauai Public Library (1967).  
Pearl City: Leeward Community College Library (1967).  
Wailuku: Maui Public Library (1962).

## IDAHO

Boise:  
Boise State College Library (1966).  
Boise Public Library (1929).  
Idaho State Law Library (unknown).  
Idaho State Library (1971).  
Caldwell: College of Idaho, Terteling Library (1930).  
Moscow: University of Idaho Library (1907)—REGIONAL.  
Pocatello: Idaho State University Library (1908).  
Rexburg: Ricks College, David O. McKay Library (1946).  
Twin Falls: College of Southern Idaho Library (1970).

## ILLINOIS

Bloomington: Illinois Wesleyan University Libraries (1964).  
Carbondale: Southern Illinois University Library (1932).  
Carlinville: Blackburn College Library (1954).  
Carterville: Shawnee Library System (1971).  
Champaign: University of Illinois Law Library, College of Law (1965).  
Charleston: Eastern Illinois University, Booth Library (1962).  
Chicago:  
Field Museum of Natural History Library (1963).  
Chicago Public Library (1876).  
Chicago State University Library (1954).  
John Crerar Library (1909).  
Loyola University of Chicago, E. M. Cudahy Memorial Library (1966).  
Newberry Library (1890).  
Northeastern Illinois University Library (1961).  
University of Chicago Law Library (1964).  
University of Chicago Library (1897).  
University of Illinois, Chicago Circle Campus Library (1957).  
Decatur: Decatur Public Library (1954).  
De Kalb: Northern Illinois University, Swen Franklin Parson Library (1960).  
Edwardsville: Southern Illinois University, Lovejoy Memorial Library (1959).  
Elsah: Principia College, Marshall Brooks Library (1957).  
Evanston: Northwestern University Library (1876).  
Freeport: Freeport Public Library (1905).  
Galesburg: Galesburg Public Library (1896).  
Jacksonville: MacMurry College, Henry Pfeiffer Library (1929).  
Kankakee: Olivet Nazarene College, Memorial Library (1946).  
Lake Forest: Lake Forest College, Donnelley Library (1962).  
Lebanon: McKendree College, Holman Library (1968).  
Lisle: Illinois Benedictine College, Theodore F. Lownik Library (1911).  
Lockport: Lewis College of Science and Technology Library (1952).  
Macomb: Western Illinois University Memorial Library (1962).

Moline: Black Hawk College, Learning Resources Center (1970).  
Monmouth: Monmouth College Library (1860).  
Normal: Illinois State University, Milner Library (1877).  
Oak Park: Oak Park Public Library (1963).  
Palos Hills: Moraine Valley Community College Library (1972).  
Peoria:  
Bradley University, Cullom Davis Library (1963).  
Peoria Public Library (1883).  
River Forest: Rosary College Library (1966).  
Rockford: Rockford Public Library (unknown).  
Springfield: Illinois State Library (unknown)—REGIONAL.  
Urbana: University of Illinois Library (1907).  
Wheaton: Wheaton College Library (1964).  
Woodstock: Woodstock Public Library (1963).

## INDIANA

Anderson: Anderson College, Charles E. Wilson Library (1959).  
Bloomington: Indiana University Library (1881).  
Crawfordsville: Wabash College, Lilly Library (1906).  
Evansville:  
Evansville and Vanderburgh County Public Library (1928).  
Indiana State University, Evansville Campus Library (1969).  
Fort Wayne:  
Indiana-Purdue Universities, Regional Campus Library (1965).  
Public Library of Fort Wayne and Allen County (1896).  
Gary:  
Gary Public Library (1943).  
Indiana University, Northwest Campus Library (1966).  
Greencastle: De Pauw University, Roy O. West Library (1879).  
Hammond: Hammond Public Library (1964).  
Hanover: Hanover College Library (1892).  
Huntington: Huntington College Library (1964).  
Indianapolis:  
Butler University, Irwin Library (1965).  
Indiana State Library (unknown)—REGIONAL.  
Indiana University, Law Library (1967).  
Indianapolis Public Library (1906).  
Jeffersonville: Indiana University, Southeastern Campus Library (1965).  
Kokomo: Indiana University, Kokomo Regional Campus Library (1969).  
Lafayette: Purdue University Library (1907).  
Muncie:  
Ball State University Library (1959).  
Muncie Public Library (1906).  
Notre Dame: University of Notre Dame, Memorial Library (1883).  
Rensselaer: St. Joseph's College Library (1964).  
Richmond:  
Earlham College, Lilly Library (1964).  
Morrison-Reeves Library (1906).  
South Bend: Indiana University at South Bend Library (1965).  
Terre Haute: Indiana State University, Cunningham Memorial Library (1906).  
Valparaiso: Valparaiso University, Moellering Memorial Library (1930).

## IOWA

Ames: Iowa State University of Science and Technology Library (1907).  
Cedar Falls: University of Northern Iowa Library (1946).  
Council Bluffs: Free Public Library (1885).  
Des Moines:  
Drake University, Cowles Library (1966).



Iowa State Traveling Library (unknown).  
Public Library of Des Moines (1888).  
Dubuque:  
Carnegie-Stout Public Library (unknown).  
Loras College, Wahlert Memorial Library (1967).  
Fairfield: Parsons College Library Branch of Fairfield Public Library (1862).  
Grinnell: Grinnell College, Burling Library (1874).  
Iowa City:  
University of Iowa, Law Library (1968).  
University of Iowa Library (1884)—REGIONAL.  
Lamoni: Graceland College, Frederick Madison Smith Library (1927).  
Mount Vernon: Cornell College, Russell D. Cole Library (1896).  
Orange City: Northwestern College, Ramaker Library (1970).  
Sioux City: Sioux City Public Library (1894).

## KANSAS

Atchison: Benedictine College Library (1965).  
Baldwin City: Baker University Library (1908).  
Colby: Colby Community Junior College Library (1968).  
Emporia: Kansas State Teachers College, William Allen White Library (1909).  
Hays: Fort Hays Kansas State College, Forsyth Library (1926).  
Hutchinson: Hutchinson Public Library (1963).  
Lawrence:  
University of Kansas, Watson Library (1869).  
University of Kansas Law Library (1971).  
Manhattan: Kansas State University, Farrell Library (1907).  
Pittsburg: Kansas State College of Pittsburg, Porter Library (1952).  
Salina: Kansas Wesleyan University, Memorial Library (1930).  
Topeka:  
Kansas State Historical Society Library (1877).  
Kansas State Library (unknown).  
Washburn University of Topeka, Law Library (1971).  
Wichita: Wichita State University Library (1901).

## KENTUCKY

Ashland: Ashland Public Library (1946).  
Barbourville: Union College, Abigail E. Weeks Memorial Library (1958).  
Bowling Green: Western Kentucky University, Cravens Graduate Center and Library (1934).  
Covington: Thomas More College Library (1970).  
Danville: Centre College, Grace Doherty Library (1884).  
Frankfort:  
Kentucky Department of Libraries (1967).  
Kentucky State University, Blazer Library (1972).  
State Law Library (unknown).  
Lexington:  
University of Kentucky, Law Library (1968).  
University of Kentucky, Margaret I. King Library (1907)—REGIONAL.  
Louisville:  
Louisville Free Public Library (1904).  
University of Louisville, Belknap Campus Library (1925).  
Morehead: Morehead State University, Johnson Camden Library (1955).  
Murray: Murray State University Library (1924).  
Owensboro: Kentucky Wesleyan College Library (1966).  
Pikeville: Pikeville College Library (1947).  
Richmond: Eastern Kentucky University, John Grant Crabbe Library (1966).

## LOUISIANA

Baton Rouge:  
Louisiana State University Law Library (1929).  
Louisiana State University Library (1907)—REGIONAL.  
Southern University Library (1952).  
Eunice: Louisiana State University at Eunice, LeDoux Library (1969).  
Hammond: Southeastern Louisiana University, Sims Memorial Library (1966).  
Lafayette: University of Southwestern Louisiana Library (1938).  
Lake Charles: McNeese State University, Frazar Memorial Library (1941).  
Monroe: Northeast Louisiana University, Sandel Library (1963).  
Natchitoches: Northwestern State College of Louisiana, Russell Library (1887).  
New Orleans:  
Isaac Delgado College, Moss Technical Library (1968).  
Law Library of Louisiana (unknown).  
Louisiana State University in New Orleans Library (1963).  
Loyola University Library (1942).  
New Orleans Public Library (1883).  
Southern University in New Orleans Library (1962).  
Tulane University, Howard-Tilton Memorial Library (1942).  
Pineville: Louisiana College, Richard W. Norton Memorial Library (1969).  
Ruston: Louisiana Technical University Library (1896)—REGIONAL.  
Shreveport:  
Louisiana State University at Shreveport Library (1967).  
Shreve Memorial Library (1923).  
Thibodaux: Francis T. Nicholls State College, Leonidas Polk Library (1962).

## MAINE

Augusta: Maine State Library (unknown).  
Bangor: Bangor Public Library (1884).  
Brunswick: Bowdoin College, Hawthorne-Longfellow Library (1884).  
Castine: Maine Maritime Academy, Nutting Memorial Library (1969).  
Lewiston: Bates College Library (1883).  
Orono: University of Maine, Raymond H. Fogler Library (1907)—REGIONAL.  
Portland:  
Portland Public Library (1884).  
University of Maine Law Library (1964).  
Springvale: Nasson College Library (1961).  
Waterville: Colby College Library (1884).

## MARYLAND

Annapolis:  
Maryland State Library (unknown).  
U.S. Naval Academy Library (1895).  
Baltimore:  
Enoch Pratt Free Library (1887).  
Johns Hopkins University, Milton S. Eisenhower Library (1882).  
Morgan State College, Soper Library (1940).  
University of Maryland, Baltimore County Library (1971).  
University of Maryland, School of Law Library (1969).  
Bel Air: Harford Community College Library (1967).  
Chestertown: Washington College, Chester M. Miller Library (1891).

College Park: University of Maryland, McKeldin Library (1925)—REGIONAL  
 Frostburg: Frostburg State College Library (1967).  
 Germantown: Atomic Energy Commission Library (1963).  
 Patuxent River: Naval Air Station Library (1968).  
 Rockville: Montgomery County Department of Public Libraries (1951).  
 Salisbury: Salisbury State College, Blackwell Library (1965).  
 Towson: Goucher College, Julia Rogers Library (1966).  
 Westminster: Western Maryland College Library (1896).

## MASSACHUSETTS

Amherst:  
 Amherst College Library (1884).  
 University of Massachusetts, Goodell Library (1907).  
 Belmont: Belmont Memorial Library (1968).  
 Boston:  
 Boston Athenaeum Library (unknown).  
 Boston College, Bapst Library (1963).  
 Boston Public Library (1859)—REGIONAL.  
 Northeastern University, Dodge Library (1962).  
 State Library of Massachusetts (unknown).  
 Brookline: Public Library of Brookline (1925).  
 Cambridge:  
 Harvard College Library (1860).  
 Massachusetts Institute of Technology Libraries (1946).  
 Chicopee: Our Lady of the Elms College Library (1969).  
 Lowell: Lowell Technological Institute, Alumni Memorial Library (1952).  
 Lynn: Lynn Public Library (1953).  
 Marlborough: Marlborough Public Library (1971).  
 Medford: Tufts University Library (1899).  
 Milton: Curry College Library (1972).  
 New Bedford: New Bedford Free Public Library (1858).  
 North Dartmouth: Southeastern Massachusetts University Library (1965).  
 North Easton: Stonehill College, Cushing-Martin Library (1962).  
 Springfield: Springfield City Library (1966).  
 Waltham: Brandeis University, Goldfarb Library (1965).  
 Wellesley: Wellesley College Library (1943).  
 Wenham: Gordon College, Winn Library (1963).  
 Williamstown: Williams College Library (unknown).  
 Wilmington: Wilmington Memorial Library (1971).  
 Worcester:  
 American Antiquarian Society Library (1814).  
 University of Massachusetts, Medical Center Library (1972).  
 Worcester Public Library (1859).

## MICHIGAN

Albion: Albion College, Stockwell Memorial Library (1966).  
 Allendale: Grand Valley State College Library (1963).  
 Alma: Alma College, Monteith Library (1963).  
 Ann Arbor:  
 Great Lakes Basin Library (1971).  
 University of Michigan, Harlan Hatcher Library (1884).  
 Battle Creek: Willard Library (1876).  
 Benton Harbor: Benton Harbor Public Library (1907).  
 Bloomfield Hills: Cranbrook Institute of Science Library (1940).  
 Dearborn:  
 Henry Ford Centennial Library (1969).  
 Henry Ford Community College Library (1957).  
 Detroit:  
 Detroit Public Library (1868)—REGIONAL.  
 Marygrove College Library (1965).

Mercy College of Detroit Library (1965).  
 University of Detroit Library (1884).  
 Wayne County Public Library (1957).  
 Wayne State University Law Library (1971).  
 Wayne State University Library (1937).  
 Dowagiac: Southwestern Michigan College Library (1971).  
 East Lansing:  
 Michigan State University, Law Library (1971).  
 Michigan State University Library (1907).  
 Escanaba: Michigan State Library, Upper Peninsula Branch (1964).  
 Farmington: Martin Luther King Learning Resources Center, Oakland Community College (1968).  
 Flint:  
 Charles Stewart Mott Library (1959).  
 Flint Public Library (1967).  
 Grand Rapids:  
 Grand Rapids Public Library (1876).  
 Calvin College Library (1967).  
 Houghton: Michigan Technological University Library (1876).  
 Jackson: Jackson Public Library (1965).  
 Kalamazoo:  
 Kalamazoo Library System (1907).  
 Western Michigan University, Dwight B. Waldo Library (1963).  
 Lansing: Michigan State Library (unknown)—REGIONAL.  
 Livonia: Schoolcraft College Library (1962).  
 Marquette: Northern Michigan University, Olsen Library (1963).  
 Mt. Clemens: Macomb County Library (1968).  
 Mt. Pleasant: Central Michigan University Library (1958).  
 Muskegon: Hackley Public Library (1894).  
 Petoskey: North Central Michigan College Library (1962).  
 Port Huron: Saint Clair County Library System (1876).  
 Rochester: Oakland University, Kresge Library (1964).  
 Saginaw: Hoyt Public Library (1890).  
 Traverse City: Northwestern Michigan College, Mark Osterlin Library (1964).  
 University Center: Delta College Library (1963).  
 Ypsilanti: Eastern Michigan University Library (1965).

## MINNESOTA

Bemidji: Bemidji State College, A. C. Clark Library (1963).  
 Collegeville: St. John's University, Alcuin Library (1954).  
 Duluth: Duluth Public Library (1909).  
 Mankato: Mankato State College Memorial Library (1962).  
 Minneapolis:  
 Anoka County Library (1971).  
 Hennepin County Library (1971).  
 Minneapolis Public Library (1893).  
 University of Minnesota, Wilson Library (1907)—REGIONAL.  
 Moorhead: Moorhead State College Library (1956).  
 Morris: University of Minnesota at Morris Library (1963).  
 Northfield:  
 Carleton College Library (1930).  
 St. Olaf College, Rolvaag Memorial Library (1930).  
 St. Cloud: St. Cloud State College Library (1962).  
 St. Paul:  
 Minnesota Historical Society Library (1867).  
 Minnesota State Law Library (unknown).  
 St. Paul Public Library (1914).  
 Saint Peter: Gustavus Adolphus College Library (1941).  
 Stillwater: Stillwater Public Library (1893).  
 Willmar: Crow River Regional Library (1958).  
 Winona: Winona State College, Maxwell Library (1969).



## MISSISSIPPI

Columbus: Mississippi State College for Women, J. C. Fant Memorial Library (1929).  
Hattiesburg: University of Southern Mississippi Library (1935).  
Jackson:  
    Jackson State College Library (1968).  
    Millsaps College, Millsaps-Wilson Library (1963).  
    Mississippi Library Commission (1947).  
    Mississippi State Law Library (unknown).  
Lorman: Alcorn Agricultural and Mechanical College Library (1970).  
State College: Mississippi State University, Mitchell Memorial Library (1907).  
University:  
    University of Mississippi Library (1883).  
    University of Mississippi, School of Law Library (1967).

## MISSOURI

Cape Girardeau: Southeast Missouri State College, Kent Library (1916).  
Columbia: University of Missouri Library (1862).  
Fayette: Central Methodist College Library (1962).  
Fulton: Westminster College, Reeves Library (1875).  
Jefferson City:  
    Lincoln University, Inman E. Page Library (1944).  
    Missouri State Library (1963).  
    Missouri Supreme Court Library (unknown).  
Joplin: Missouri Southern State College Library (1966).  
Kansas City:  
    Kansas City Public Library (1881).  
    Rockhurst College Library (1917).  
    University of Missouri at Kansas City, General Library (1938).  
Kirkville: Northeast Missouri State Teachers College, Pickler Memorial Library (1966).  
Liberty: William Jewell College Library (1900).  
Rolla: University of Missouri at Rolla Library (1907).  
St. Joseph: St. Joseph Public Library (1891).  
St. Louis:  
    St. Louis County Library (1970).  
    St. Louis Public Library (1866).  
    St. Louis University, Law Library (1967).  
    St. Louis University, Pius XII Memorial Library (1866).  
    University of Missouri at St. Louis, Thomas Jefferson Library (1966).  
    Washington University, John M. Olin Library (1906).  
Springfield:  
    Drury College, Walker Library (1874).  
    Southwest Missouri State College Library (1963).  
Warrensburg: Central Missouri State College, Ward Edwards Library (1914).

## MONTANA

Billings: Eastern Montana College Library (1924).  
Bozeman: Montana State University Library (1907).  
Butte: Montana College of Mineral Science and Technology Library (1901).  
Helena:  
    Montana Historical Society Library (unknown).  
    Montana State Library (1966).  
Missoula: University of Montana Library (1909)–REGIONAL.

## NEBRASKA

Blair: Dana College, Dana-LIFE Library (1924).  
Crete: Doane College, Whitin Library (1944).  
Fremont: Midland Lutheran College Library (1924).  
Kearney: Kearney State College, Calvin T. Ryan Library (1962).  
Lincoln:  
    Nebraska Publications Clearinghouse, Nebraska Library Commission (1972).  
    Nebraska State Library (unknown).  
    University of Nebraska, Don L. Love Memorial Library (1907).  
Omaha:  
    Creighton University, Alumni Library (1964).  
    Omaha Public Library (1880).  
    University of Nebraska at Omaha, Gene Eppley Library (1939).  
Scottsbluff: Scottsbluff Public Library (1925).  
Wayne: Wayne State College, U.S. Conn Library (1970).

## NEVADA

Carson City: Nevada State Library (unknown).  
Las Vegas: University of Nevada at Las Vegas, James R. Dickinson Library (1959).  
Reno: University of Nevada Library (1907)–REGIONAL

## NEW HAMPSHIRE

Concord: New Hampshire State Library (unknown).  
Durham: University of New Hampshire Library (1907).  
Franconia: Franconia College Library (1972).  
Hanover: Dartmouth College, Baker Library (1884).  
Henniker: New England College Library (1966).  
Manchester:  
    Manchester City Library (1884).  
    St. Anselm's College, Geisel Library (1963).  
Nashua: Nashua Public Library (1971).

## NEW JERSEY

Bayonne: Bayonne Free Public Library (1909).  
Bloomfield: Free Public Library of Bloomfield (1965).  
Bridgeton: Cumberland County Library (1966).  
Camden: Rutgers University-Camden Library (1966).  
Convent Station: College of St. Elizabeth, Mahoney Library (1938).  
East Orange: East Orange Public Library (1966).  
Elizabeth: Free Public Library of Elizabeth (1895).  
Glassboro: Glassboro State College, Savitz Learning Resource Center (1963).  
Hackensack: Johnson Free Public Library (1966).  
Irvington: Free Public Library of Irvington (1966).  
Jersey City:  
    Free Public Library of Jersey City (1879).  
    Jersey City State College, Forrest A. Irwin Library (1963).  
Madison: Drew University, Rose Memorial Library (1939).  
Mahwah: Ramapo College Library (1971).  
Mount Holly: Burlington County Library (1966).  
New Brunswick:  
    Free Public Library (1908).  
    Rutgers University Library (1907).  
Newark:  
    Newark Public Library (1906)–REGIONAL.  
    Rutgers-The State University, John Cotton Dana Library (1966).  
Passaic: Passaic Public Library (1964).

Plainfield: Plainfield Public Library (1971).  
 Pomona: Stockton State College Library (1972).  
 Princeton: Princeton University Library (1884).  
 Rutherford: Fairleigh Dickinson University, Messler Library (1953).  
 Shrewsbury: Monmouth County Library (1968).  
 South Orange: Seton Hall University Library (1947).  
 Teaneck: Fairleigh Dickinson University, Teaneck Campus Library (1963).  
 Toms River: Ocean County College Learning Resources Center (1966).  
 Trenton:  
     New Jersey State Library, Law and Reference Bureau, Department of Education (unknown).  
     Trenton Free Public Library (1902).  
 Upper Montclair: Montclair State College, Harry A. Sprague Library (1967).  
 Wayne: Wayne Public Library (1972).  
 West Long Branch: Monmouth College, Guggenheim Memorial Library (1963).  
 Woodbridge: Free Public Library of Woodbridge (1965).

## NEW MEXICO

Albuquerque: University of New Mexico, Zimmerman Library (1896) – REGIONAL.  
 Hobbs: New Mexico Junior College, Pannell Library (1969).  
 Las Cruces: New Mexico State University Library (1907).  
 Las Vegas: New Mexico Highlands University, Donnelly Library (1913).  
 Portales: Eastern New Mexico University Library (1962).  
 Santa Fe:  
     New Mexico State Library (1960) – REGIONAL.  
     Supreme Court Law Library (unknown).

## NEW YORK

Albany:  
     New York State Library (unknown) – REGIONAL.  
     State University of New York at Albany Library (1964).  
 Auburn: Seymour Library (1972).  
 Bayside: Queensborough Community College Library (1972).  
 Binghamton: State University of New York at Binghamton Library (1962).  
 Brockport: State University of New York, Drake Memorial Library (1967).  
 Bronx: Herbert H. Lehman College Library (1967).  
 Bronxville: Sarah Lawrence College Library (1969).  
 Brooklyn:  
     Brooklyn College Library (1936).  
     Brooklyn Public Library (1908).  
     Polytechnic Institute of Brooklyn, Spicer Library (1963).  
     Pratt Institute Library (1891).  
     State University of New York, Downstate Medical Center Library (1958).  
 Buffalo:  
     Buffalo and Erie County Public Library (1895).  
     State University of New York at Buffalo, Lockwood Memorial Library (1963).  
 Canton: St. Lawrence University, Owen D. Young Library (1920).  
 Corning: Corning Community College, Arthur A. Houghton, Jr. Library (1963).  
 Cortland: State University of New York, College at Cortland, Memorial Library (1964).  
 Delhi: State University Agricultural and Technical College Library (1970).  
 Douglaston: Cathedral College Library (1971).

Elmira: Elmira College, Gannett-Tripp Learning Center (1956).  
 Farmingdale: State University Agricultural and Technical Institute at Farmingdale Library (1917).  
 Flushing: Queens College, Paul Klapper Library (1939).  
 Garden City:  
     Adelphi University, Swirbul Library (1966).  
     Nassau Library System (1965).  
 Geneseo: State University College, Milne Library (1967).  
 Greenvale: C. W. Post College, B. Davis Schwartz Memorial Library (1964).  
 Hamilton: Colgate University Library (1902).  
 Hempstead: Hofstra University Library (1964).  
 Huntington: Huntington Public Library (1966).  
 Ithaca:  
     Cornell University Library (1907).  
     New York State Colleges of Agriculture and Home Economics, Albert R. Mann Library (1943).  
 Jamaica:  
     Queens Borough Public Library (1926).  
     St. John's University Library (1956).  
 Kings Point: U.S. Merchant Marine Academy Library (1962).  
 Mount Vernon: Mount Vernon Public Library (1962).  
 New Paltz: State University College Library (1965).  
 New York City:  
     City University of New York, City College Library (1884).  
     College of Insurance, Ecker Library (1965).  
     Columbia University Libraries (1882).  
     Cooper Union Library (1930).  
     Fordham University Library (1937).  
     New York Law Institute Library (1909).  
     New York Public Library (Astor Branch) (1907).  
     New York Public Library (Lenox Branch) (1884).  
     New York University Libraries (1967).  
     New York University, University Heights Gould Memorial Library (1902).  
     State University of New York, Maritime College Library (1947).  
 Newburgh: Newburgh Free Library (1909).  
 Oakdale: Dowling College Library (1965).  
 Oneonta: State University College, James M. Milne Library (1966).  
 Oswego: State University College, Penfield Library (1966).  
 Plattsburgh: State University College, Benjamin F. Feinberg Library (1967).  
 Potsdam:  
     Clarkson College of Technology, Harriet Call Burnap Memorial Library (1938).  
     State University College, Frederick W. Crumb Memorial Library (1964).  
 Poughkeepsie: Vassar College Library (1943).  
 Purchase: State University of New York, College at Purchase Library (1969).  
 Rochester:  
     Rochester Public Library (1963).  
     University of Rochester Library (1880).  
 St. Bonaventure: St. Bonaventure College, Friedsam Memorial Library (1938).  
 Saratoga Springs: Skidmore College Library (1964).  
 Schenectady: Union College, Schaffer Library (1901).  
 Staten Island (Grymes Hill): Wagner College, Horrmann Library (1953).  
 Stony Brook: State University of New York at Stony Brook Library (1963).  
 Syracuse: Syracuse University Library (1878).  
 Troy: Troy Public Library (1869).  
 Utica: Utica Public Library (1885).  
 West Point: U.S. Military Academy Library (unknown).  
 Yonkers: Yonkers Public Library (1910).



## NORTH CAROLINA

- Asheville: University of North Carolina at Asheville, D. Hiden Ramsey Library (1965).  
 Boone: Appalachian State University Library (1963).  
 Buies Creek: Campbell College, Carrie Rich Memorial Library (1965).  
 Chapel Hill: University of North Carolina Library (1884) — REGIONAL.  
 Charlotte:  
     Public Library of Charlotte and Mecklenburg County (1964).  
     Queens College, Everett Library (1927).  
     University of North Carolina at Charlotte, Atkins Library (1964).  
 Cullowhee: Western Carolina University, Hunter Library (1953).  
 Davidson: Davidson College, Hugh A. & Jane Grey Memorial Library (1893).  
 Durham: Duke University, William R. Perkins Library (1890).  
 Elon College: Elon College Library (1971).  
 Fayetteville: Fayetteville State University, Chestnut Library (1971).  
 Greensboro:  
     North Carolina Agricultural and Technical State University, F. D. Bluford Library (1937).  
     University of North Carolina at Greensboro, Walter Clinton Jackson Library (1963).  
 Greenville: East Carolina University, J. Y. Joyner Library (1951).  
 Laurinburg: St. Andrews Presbyterian College, DeTamble Library (1969).  
 Lexington: Davidson County Public Library System (1971).  
 Mount Olive: Mount Olive College, Moye Library (1971).  
 Murfreesboro: Chowan College, Whitaker Library (1963).  
 Pembroke: Pembroke State University Library (1965).  
 Raleigh:  
     North Carolina State Library (unknown).  
     North Carolina State University, D. H. Hill Library (1923).  
     Wake County Public Libraries (1969).  
 Rocky Mount: North Carolina Wesleyan College Library (1969).  
 Salisbury: Catawba College Library (1925).  
 Wilmington: University of North Carolina at Wilmington, William M. Randall Library (1965).  
 Wilson: Atlantic Christian College, Clarence L. Hardy Library (1930).  
 Winston-Salem:  
     Forsyth County Public Library System (1954).  
     Wake Forest University, Z. Smith Reynolds Library (1902).

## NORTH DAKOTA

- Bismarck:  
     State Historical Society of North Dakota (1907).  
     North Dakota State Law Library (unknown).  
     State Library Commission Library (1971).  
     Veterans Memorial Public Library (1967).  
 Dickinson: Dickinson State College Library (1968).  
 Fargo:  
     Fargo Public Library (1964).  
     North Dakota State University Library (1907) — REGIONAL, in cooperation with University of North Dakota, Chester Fritz Library at Grand Forks.  
 Grand Forks: University of North Dakota, Chester Fritz Library (1890).  
 Minot: Minot State College, Memorial Library (1925).  
 Valley City: State College Library (1913).

## OHIO

- Ada: Ohio Northern University, J. P. Taggart Law Library (1965).  
 Akron:  
     Akron Public Library (1952).  
     University of Akron Library (1963).  
 Alliance: Mount Union College Library (1888).  
 Ashland: Ashland College Library (1938).  
 Athens: Ohio University Library (1886).  
 Bluffton: Bluffton College, Musselman Library (1951).  
 Bowling Green: Bowling Green State University Library (1933).  
 Canton: Malone College, Everett L. Cattell Library (1970).  
 Chardon: Geauga County Public Library (1971).  
 Cincinnati:  
     Public Library of Cincinnati and Hamilton County (1884).  
     University of Cincinnati Library (1929).  
 Cleveland:  
     Case Western Reserve University, Freiburger Library (1913).  
     Cleveland Heights-University Heights Public Library (1970).  
     Cleveland Public Library (1886).  
     Cleveland State University Library (1966).  
     John Carroll University, Grasselli Library (1963).  
     Municipal Reference Library (1970).  
 Columbus:  
     Capital University Library (1968).  
     Columbus Public Library (1885).  
     Ohio State Library (unknown) — REGIONAL.  
     Ohio State University Library (1907).  
 Dayton:  
     Dayton and Montgomery County Public Library (1909).  
     University of Dayton, Albert Emanuel Library (1969).  
     Wright State University Library (1965).  
 Delaware: Ohio Wesleyan University, L. A. Beeghly Library (1845).  
 Elyria: Elyria Public Library (1966).  
 Findlay: Findlay College, Shafer Library (1969).  
 Gambier: Kenyon College Library (1873).  
 Granville: Denison University Library (1884).  
 Hiram: Hiram College, Teachout-Price Memorial Library (1874).  
 Kent: Kent State University Library (1962).  
 Marietta: Marietta College, Dawes Memorial Library (1884).  
 Middletown: Miami University at Middletown, Gardner-Harvey Library (1970).  
 New Concord: Muskingum College Library (1966).  
 Oberlin: Oberlin College Library (1958).  
 Oxford: Miami University, Alumni Library (1909).  
 Portsmouth: Portsmouth Public Library (unknown).  
 Rio Grande: Rio Grande College, Jeanette Albiez Davis Library (1966).  
 Springfield: Warder Public Library (1884).  
 Steubenville:  
     College of Steubenville, Starvaggi Memorial Library (1971).  
     Public Library of Steubenville and Jefferson County (1950).  
 Tiffin: Heidelberg College, Beeghly Library (1964).  
 Toledo:  
     Toledo-Lucas County Public Library (1884).  
     University of Toledo Library (1963).  
 Westerville: Otterbein College, Centennial Library (1967).  
 Wooster: College of Wooster, The Andrews Library (1966).  
 Youngstown:  
     Public Library of Youngstown and Mahoning County (1923).  
     Youngstown State University Library (1971).

## OKLAHOMA

Ada: East Central State College, Linscheid Library (1914).  
Alva: Northwestern State College Library (1907).  
Bartlesville: Bureau of Mines, Petroleum Research Center Library (1962).  
Bethany: Bethany Nazarene College, R. T. Williams Library (1971).  
Durant: Southeastern State College Library (1929).  
Edmond: Central State University Library (1934).  
Enid: Public Library of Enid and Garfield County (1908).  
Langston: Langston University, G. Lamar Harrison Library (1941).  
Muskogee: Muskogee Public Library (1971).  
Norman: University of Oklahoma Libraries (1893).  
Oklahoma City:  
    Oklahoma City University Library (1963).  
    Oklahoma Department of Libraries (1893)—REGIONAL.  
Shawnee: Oklahoma Baptist University Library (1933).  
Stillwater: Oklahoma State University Library (1907).  
Tahlequah: Northeastern State College, John Vaughan Library (1923).  
Tulsa:  
    Tulsa City-County Library Commission (1963).  
    University of Tulsa, McFarlin Library (1929).  
Weatherford: Southwestern State College Library (1958).

## OREGON

Ashland: Southern Oregon College Library (1953).  
Corvallis: Oregon State University Library (1907).  
Eugene: University of Oregon Library (1883).  
Forest Grove: Pacific University Library (1897).  
La Grande: Eastern Oregon College, Walter M. Pierce Library (1954).  
McMinnville: Linfield College, Northup Library (1965).  
Monmouth: Oregon College of Education Library (1967).  
Portland:  
    Department of the Interior, Bonneville Power Administration Library (1962).  
    Lewis and Clark College, Aubrey R. Watzek Library (1967).  
    Library Association of Portland (1884).  
    Portland State University Library (1963)—REGIONAL.  
    Reed College Library (1912).  
Salem:  
    Oregon State Library (unknown).  
    Willamette University Library (1969).

## PENNSYLVANIA

Allentown: Muhlenberg College, Haas Library (1939).  
Altoona: Altoona Public Library (1969).  
Bethlehem: Lehigh University, Linderman Library (1876).  
Carlisle: Dickinson College, Boyd Lee Spahr Library (1947).  
Cheyney: Cheyney State College, Leslie Pinckney Hill Library (1947).  
Collegeville: Ursinus College, Myrin Library (1963).  
Doylestown: Bucks County Free Library, Center County Library (1970).  
East Stroudsburg: East Stroudsburg State College, Kemp Library (1966).  
Erie: Erie Public Library (1897).  
Greenville: Thiel College, Langenheim Memorial Library (1963).  
Harrisburg: State Library of Pennsylvania (unknown)—REGIONAL.  
Haverford: Haverford College Library (1897).

Hazleton: Hazleton Area Public Library (1964).  
Indiana: Indiana University of Pennsylvania, Rhodes R. Stabley Library (1962).  
Johnstown: Cambria Public Library (1965).  
Lancaster: Franklin and Marshall College, Fackenthal Library (1895).  
Lewisburg: Bucknell University, Ellen Clarke Bertrand Library (1963).  
Mansfield: Mansfield State College Library (1968).  
Meadville: Allegheny College, Reis Library (1907).  
Millersville: Millersville State College, Ganser Library (1966).  
Monessen: Monessen Public Library (1969).  
New Castle: New Castle Free Public Library (1963).  
Newtown: Bucks County Community College Library (1968).  
Norristown: Montgomery County-Norristown Public Library (1969).  
Philadelphia:  
    Drexel University Library (1963).  
    Free Library of Philadelphia (1897).  
    Temple University, Samuel Paley Library (1947).  
    University of Pennsylvania Library (1886).  
Pittsburgh:  
    Bureau of Mines, Pittsburgh Research Center Library (1962).  
    Carnegie Library of Pittsburgh, Allegheny Regional Branch (1924).  
    Carnegie Library of Pittsburgh (1895).  
    University of Pittsburgh, Hillman Library (1910).  
Pottsville: Pottsville Free Public Library (1967).  
Reading: Reading Public Library (1901).  
Scranton: Scranton Public Library (1895).  
Slippery Rock: Slippery Rock State College, Maltby Library (1965).  
Swarthmore: Swarthmore College Library (1923).  
University Park: Pennsylvania State University Library (1907).  
Villanova: Villanova University, School of Law Library (1964).  
Warren: Warren Library Association, Warren Public Library (1885).  
Washington: Washington and Jefferson College, Memorial Library (1884).  
Waynesburg: Waynesburg College Library (1964).  
West Chester: West Chester State College, Francis Harvey Green Library (1967).  
Wilkes-Barre: King's College, Corgan Library (1949).  
Williamsport: Lycoming College Library (1970).  
York: York Junior College Library (1963).

## PUERTO RICO

Mayaguez: University of Puerto Rico, Mayaguez Campus Library (1928).  
Ponce: Catholic University of Puerto Rico Library (1966).  
Rio Piedras: University of Puerto Rico General Library (1928).

## RHODE ISLAND

Kingston: University of Rhode Island Library (1907).  
Newport: Naval War College Library (1963).  
Providence:  
    Brown University, John D. Rockefeller, Jr. Library (unknown).  
    Providence College, Phillips Memorial Library (1969).  
    Providence Public Library (1884).  
    Rhode Island College Library (1965).  
    Rhode Island State Library (before 1895).  
Warwick: Warwick Public Library (1966).  
Westerly: Westerly Public Library (1909).



## **SOUTH CAROLINA**

### **Charleston:**

Baptist College at Charleston Library (1967).  
College of Charleston Library (1869).  
The Citadel Memorial Library (1962).

### **Clemson:** Clemson University Library (1893).

### **Columbia:**

Benedict College, Starks Library (1969).  
Columbia College Library (1966).  
South Carolina State Library (before 1895).  
University of South Carolina Undergraduate Library (1884).

### **Due West:** Erskine College, McCain Library (1968).

### **Florence:**

Florence County Library (1967).  
Francis Marion College, James A. Rogers Library (1970).

### **Greenville:**

Furman University Library (1962).  
Greenville County Library (1966).

### **Greenwood:** Lander College Library (1967).

### **Orangeburg:** South Carolina State College, Whittaker Library (1953).

### **Rock Hill:** Winthrop College Library (1896).

### **Spartanburg:** Spartanburg County Public Library (1967).

## **SOUTH DAKOTA**

### **Aberdeen:** Northern State College Library (1963).

### **Brookings:** South Dakota State University, Lincoln Memorial Library (1889).

### **Rapid City:**

Rapid City Public Library (1963).  
South Dakota School of Mines and Technology Library (1963).

### **Sioux Falls:**

Augustana College, Mikkelsen Library and Learning Resources Center (1969).  
Carnegie Free Public Library (1903).

### **Spearfish:** Black Hills State College Library (1942).

### **Vermillion:** University of South Dakota, I. D. Weeks Library (1889).

### **Yankton:** Yankton College, Corliss Lay Library (1904).

## **TENNESSEE**

### **Bristol:** King College Library (1970).

### **Chattanooga:** Chattanooga Public Library (1907).

### **Clarksville:** Austin Peay State University, Felix G. Woodward Library (1945).

### **Cookeville:** Tennessee Technological University, Jere Whitson Memorial Library (1969).

### **Jackson:** Lambuth College, Luther L. Gobbel Library (1967).

### **Jefferson City:** Carson-Newman College Library (1964).

### **Johnson City:** East Tennessee State University, Sherrod Library (1942).

### **Knoxville:**

University of Tennessee Law Library (1971).  
University of Tennessee Library (1907).

### **Martin:** University of Tennessee at Martin Library (1957).

### **Memphis:**

Memphis Public Library and Information Center (1896).  
Memphis State University, John W. Brister Library (1966).

### **Morristown:** Morristown College, Carnegie Library (1970).

### **Murfreesboro:** Middle Tennessee State University, Andrew L. Todd Library (1912).

### **Nashville:**

Fisk University Library (1965).

### **Joint University Libraries** (1884).

### **Public Library of Nashville and Davidson County** (1884).

### **Tennessee State Library and Archives, State Library Division** (unknown).

### **Tennessee State University, Martha M. Brown Memorial Library** (1972).

### **Sewanee:** University of the South, Jesse Ball duPont Library (1873).

## **TEXAS**

### **Abilene:** Hardin-Simmons University Library (1940).

### **Arlington:**

Arlington Public Library (1970).  
University of Texas at Arlington Library (1963).

### **Austin:**

Texas State Library (unknown)—REGIONAL.  
University of Texas at Austin Library (1884).  
University of Texas, Lyndon B. Johnson School of Public Affairs Library (1966).  
University of Texas, School of Law Library (1965).

### **Baytown:** Lee College Library (1970).

### **Beaumont:** Lamar University Library (1957).

### **Brownwood:** Howard Payne College, Walker Memorial Library (1964).

### **Canyon:** West Texas State University Library (1928).

### **College Station:** Texas Agricultural and Mechanical University Library (1907).

### **Commerce:** East Texas State University Library (1937).

### **Corsicana:** Navarro Junior College Library (1965).

### **Dallas:**

Bishop College, Zale Library (1966).  
Dallas Baptist College Library (1967).  
Dallas Public Library (1900).  
Southern Methodist University, Fondren Library (1925).  
University of Texas at Dallas Library (1972).

### **Denton:** North Texas State University Library (1948).

### **Edinburg:** Pan American University Library (1959).

### **El Paso:**

El Paso Public Library (1906).  
University of Texas at El Paso Library (1966).

### **Fort Worth:**

Fort Worth Public Library (1905).  
Texas Christian University, Mary Coats Burnett Library (1916).

### **Galveston:** Rosenberg Library (1909).

### **Houston:**

Houston Public Library (1884).  
Rice University, Fondren Library (1967).  
University of Houston Library (1957).

### **Huntsville:** Sam Houston State University, Estill Library (1949).

### **Kingsville:** Texas Arts and Industries University Library (1944).

### **Lake Jackson:** Brazosport College Library (1969).

### **Laredo:** Laredo Junior College Library (1970).

### **Longview:** Nicholson Memorial Public Library (1961).

### **Lubbock:** Texas Tech University Library (1935)—REGIONAL.

### **Marshall:** Wiley College, Cole Library (1962).

### **Nacogdoches:** Stephen F. Austin State University Library (1965).

### **Plainview:** Wayland Baptist College, Van Howeling Memorial Library (1963).

### **San Angelo:** Angelo State University, Porter Henderson Library (1964).

### **San Antonio:**

San Antonio College Library (1972).

San Antonio Public Library, Business and Science Department (1899).  
 St. Mary's University Library (1964).  
 Trinity University Library (1964).  
 San Marcos: Southwest Texas State University Library (1955).  
 Seguin: Texas Lutheran College, Blumberg Memorial Library (1970).  
 Sherman: Austin College, Arthur Hopkins Library (1963).  
 Texarkana: Texarkana Community College, Palmer Memorial Library (1963).  
 Waco: Baylor University Library (1905).  
 Wichita Falls: Midwestern University, Moffett Library (1963).

## UTAH

Cedar City: Southern Utah State College Library (1964).  
 Ephraim: Snow College, Lucy A. Phillips Library (1963).  
 Logan: Utah State University, Merrill Library and Learning Resources Center (1907)—REGIONAL.  
 Ogden: Weber State College Library (1962).  
 Provo:  
   Brigham Young University Library (1908).  
   Brigham Young University Law Library (1972).  
 Salt Lake City:  
   University of Utah, Law Library (1966).  
   University of Utah, Eccles Medical Sciences Library (1970).  
   University of Utah, Marriott Library (1893).  
   Utah State Library Commission, Documents Library (unknown).

## VERMONT

Burlington: University of Vermont, Bailey Library (1907).  
 Castleton: Castleton State College, Calvin Coolidge Library (1969).  
 Johnson: Johnson State College, John Dewey Library (1955).  
 Lyndonville: Lyndon State College, Samuel Reed Hall Library (1969).  
 Middlebury: Middlebury College, Egbert Starr Library (1884).  
 Montpelier: Vermont Department of Libraries (before 1895).  
 Northfield: Norwich University Library (1908).  
 Putney: Windham College, Dorothy Culbertson Marvin Memorial Library (1965).

## VIRGIN ISLANDS

Charlotte Amalie (St. Thomas): St. Thomas Public Library (1968).

## VIRGINIA

Blacksburg: Virginia Polytechnic Institute, Newman Library (1907).  
 Bridgewater: Bridgewater College, Alexander Mack Memorial Library (1902).  
 Charlottesville:  
   University of Virginia, Alderman Library (1910)—REGIONAL.  
   University of Virginia Law Library (1964).  
 Chesapeake: Chesapeake Public Library System (1970).  
 Danville: Danville Community College Library (1969).  
 Emory: Emory and Henry College Library (1884).  
 Fairfax: George Mason College of the University of Virginia, Fenwick Library (1960).  
 Fredericksburg: Mary Washington College, E. Lee Trinkle Library (1940).

Hampden-Sydney: Hampden-Sydney College, Eggleston Library (1891).  
 Hollins College: Hollins College, Fishburn Library (1967).  
 Lexington:  
   Virginia Military Institute, Preston Library (1874).  
   Washington and Lee University, Cyrus Hall McCormick Library (1910).  
 Martinsville: Patrick Henry Community College Library (1971).  
 Norfolk:  
   Armed Forces Staff College Library (1963).  
   Norfolk Public Library (1895).  
   Old Dominion University, Hughes Memorial Library (1963).  
 Petersburg: Virginia State College, Johnston Memorial Library (1907).  
 Quantico: Marine Corps Schools, James Carson Breckinridge Library (1967).  
 Richmond:  
   University of Richmond, Boatwright Memorial Library (1900).  
   Virginia Commonwealth University, James Branch Cabell Library (1971).  
   Virginia State Library (unknown).  
 Roanoke: Roanoke Public Library (1964).  
 Salem: Roanoke College Library (1886).  
 Williamsburg: William and Mary College Library (1936).  
 Wise: Clinch Valley College, John Cook Wyllie Library (1971).

## WASHINGTON

Bellingham: Western Washington State College, Wilson Library (1963).  
 Cneney: Eastern Washington State College Library (1966).  
 Ellensburg: Central Washington State College Library (1962).  
 Everett: Everett Public Library (1914).  
 Olympia:  
   Evergreen State College Library (1972).  
   Washington State Library (unknown)—REGIONAL.  
 Port Angeles: Port Angeles Public Library (1965).  
 Pullman: Washington State University Library (1907).  
 Seattle:  
   Seattle Public Library (1908).  
   University of Washington Library (1890).  
   University of Washington, School of Law Library (1969).  
 Spokane: Spokane Public Library (1910).  
 Tacoma:  
   Tacoma Public Library (1894).  
   University of Puget Sound, Collins Memorial Library (1938).  
 Vancouver: Fort Vancouver Regional Library (1962).  
 Walla Walla: Whitman College, Penrose Memorial Library (1890).

## WEST VIRGINIA

Athens: Concord College Library (1924).  
 Bluefield: Bluefield State College Library (1972).  
 Charleston:  
   Kanawha County Public Library (1952).  
   West Virginia Department of Archives and History Library (unknown).  
 Elkins: Davis and Elkins College Library (1913).  
 Fairmont: Fairmont State College Library (1884).  
 Glenville: Glenville State College, Robert F. Kidd Library (1966).  
 Huntington: Marshall University Library (1925).  
 Institute: West Virginia State College Library (1907).



Morgantown: West Virginia University Library (1907)—REGIONAL.

Salem: Salem College Library (1921).

Shepherdstown: Shepherd College Library (1971).

Weirton: Mary H. Weir Public Library (1963).

## WISCONSIN

Appleton: Lawrence University, Samuel Appleton Library (1869).

Beloit: Beloit College Libraries (1888).

Eau Claire: University of Wisconsin, Eau Claire, William D. McIntyre Library (1951).

Fond du Lac: Fond du Lac Public Library (1966).

Green Bay: University of Wisconsin at Green Bay Library (1968).

La Crosse:

La Crosse Public Library (1883).

University of Wisconsin-La Crosse, Murphy Library (1965).

Madison:

Department of Public Instruction, Division for Library Services, Reference and Loan Library (1965).

Madison Public Library (1965).

State Historical Society Library (1870)—REGIONAL, in cooperation with University of Wisconsin, Memorial Library.

University of Wisconsin, Memorial Library (1939).

Wisconsin State Library (unknown).

Milwaukee:

Alverno College Library (1971).

Milwaukee County Law Library (1934).

Milwaukee Public Library (1961)—REGIONAL.

Mount Mary College Library (1964).

Oklahoma Neighborhood Library (1965).

University of Wisconsin-Milwaukee Library (1960).

Oshkosh: University of Wisconsin-Oshkosh, Forrest R. Polk Library (1956).

Platteville: University of Wisconsin-Platteville, Elton S. Karmann Library (1964).

Racine: Racine Public Library (1898).

River Falls: University of Wisconsin-River Falls, Chalmer Davee Library (1962).

Stevens Point: University of Wisconsin-Stevens Point, Learning Resources Center (1951).

Superior:

Superior Public Library (1908).

University of Wisconsin-Superior, Jim Dan Hill Library (1935).

Waukesha: Waukesha Public Library (1966).

Wausau: Wausau Public Library (1971).

Whitewater: Wisconsin State University, Harold Andersen Library (1963).

## WYOMING

Casper: Natrona County Public Library (1929).

Cheyenne: Wyoming State Library (unknown).

Laramie: University of Wyoming, Coe Library (1907).

Powell: Northwest Community College Library (1967).

Riverton: Central Wyoming College Library (1969).

Rock Springs: Western Wyoming College Library (1969).

Sheridan: Sheridan College, Mary Brown Kooi Library (1963).





## APPENDIX B. LIST OF FIELD OFFICES OF THE U.S. DEPARTMENT OF COMMERCE

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450 Golden Gate Avenue  
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U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET	1. PUBLICATION OR REPORT NO. NBS-SP-305, Suppl. 4	2. Gov't Accession No.	3. Recipient's Accession No.				
4. TITLE AND SUBTITLE  Publications of the National Bureau of Standards 1972 Catalog	5. Publication Date July 1973		6. Performing Organization Code				
	8. Performing Organization						
7. AUTHOR(S) Betty L. Oberholtzer	10. Project/Task/Work Unit No.		11. Contract/Grant No.				
	13. Type of Report & Period Covered 1972						
9. PERFORMING ORGANIZATION NAME AND ADDRESS  NATIONAL BUREAU OF STANDARDS DEPARTMENT OF COMMERCE WASHINGTON, D.C. 20234	14. Sponsoring Agency Code		15. SUPPLEMENTARY NOTES				
	12. Sponsoring Organization Name and Address  Same as item 9						
16. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)  This supplement to Special Publication 305 Supplements 1, 2, and 3 of the National Bureau of Standards lists the publications of the Bureau issued between January 1, 1972 and December 31, 1972. It includes an abstract of each publication (plus some earlier papers omitted from special Publication 305 Supplement 3), key-word and author indexes; and general information and instructions about NBS publications.  Miscellaneous Publication 240 (covering the period July 1, 1957 through June 30, 1960) and its supplement (covering the period July 1, 1960 through June 30, 1966), Special Publication 305 (covering the period July 1966 through December 1967) and Special Publication 305 Supplement 1 (covering the period 1968-1969), Special Publication 305 Supplement 2 (covering the period 1970), and Special Publication 305 Supplement 3 (covering the period 1971) remain in effect. Two earlier lists, Circular 460 (Publications of the National Bureau of Standards, 1901 to June 1947) and its supplement (Supplementary List of Publications of the National Bureau of Standards, July 1, 1947 to June 30, 1957) are also still in effect.							
17. KEY WORDS (Alphabetical order, separated by semicolons) Abstracts, NBS publications; key words; publications.							
18. AVAILABILITY STATEMENT  <input checked="" type="checkbox"/> UNLIMITED.  <input type="checkbox"/> FOR OFFICIAL DISTRIBUTION. DO NOT RELEASE TO NTIS.	19. SECURITY CLASS (THIS REPORT)  UNCLASSIFIED	21. NO. OF PAGES  449					
	20. SECURITY CLASS (THIS PAGE)  UNCLASSIFIED	22. Price  \$3.75					





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