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Technical Activities 1982
Office of Standard Reference Data

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
National Measurement Laboratory
Washington, DC 20234

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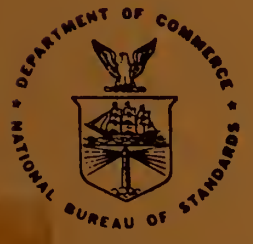

U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

NBSIR 83-2661

TECHNICAL ACTIVITIES 1983
OFFICE OF STANDARD REFERENCE DATA

S. P. Fivozinsky, Editor

U.S. DEPARTMENT OF COMMERCE
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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

ABSTRACT

The Office of Standard Reference Data is one of four program offices in the National Measurement Laboratory, National Bureau of Standards. The Standard Reference Data Program develops and disseminates data bases of critically evaluated physical/chemical properties of substances. These data bases are available through NBS and private publications, on magnetic tape, and from on-line retrieval systems.

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1982.

Key words: data compilation; energy and environmental data, evaluated data; materials data; standard reference data; technical activities 1982; thermochemical and thermophysical data

TABLE OF CONTENTS

APPENDICES

INTRODUCTION

The Office of Standard Reference Data is responsible for program management and coordination of the National Standard Reference Data System (NSRDS). The major aim of the program is to provide critically evaluated numerical data to the scientific and technical community in a convenient and accessible form. Certain secondary outputs, such as annotated bibliographies and procedures for computerized handling of data, are also made available. A second aim is to provide feedback into experimental programs to help raise the general standards of measurement. That is, by communicating the experience gained in evaluating the world output of data in the physical sciences, NSRDS helps to advance the level of experimental techniques and improve the reliability of physical measurements.

The formal existence of the NSRDS dates from 1963, when the Federal Council for Science and Technology asked the National Bureau of Standards to assume primary responsibility in the Federal Government for promoting and coordinating the critical evaluation of numerical data in the physical sciences. The program was conceived as a decentralized national effort, with financial support coming from a variety of Government and private sources, but with NBS responsible for the overall planning and coordination. In 1968 the Congress provided a specific legislative mandate for the program through passage of Public Law 90-396, the Standard Reference Data Act.* This act states the policy of the Congress to make reliable reference data available to scientists, engineers, and the general public, and it encourages cooperation among NBS, other Federal Agencies, and the private sector in meeting this objective.

The technical scope of the program gives primary emphasis to well-defined physical and chemical properties of substances and systems which are well characterized. Also included are materials of commerce (alloys, ceramics, etc.) whose composition may vary only within clearly stated ranges. Materials of uncertain or widely variable composition are not included. Properties which depend upon arbitrarily defined characteristics of the measurement technique are generally excluded. While these definitions leave many borderline cases, the overall intent is to concentrate the effort on intrinsic properties that are clearly defined in terms of accepted physical theory and substances whose composition and history are so well known as to justify evaluation of the data. Biological properties and data relating to large natural systems (e.g., the atmosphere, the oceans) also fall outside the program.

The Office of Standard Reference Data monitors and coordinates the work of the various data centers and specialized projects which collectively make up the NSRDS. These projects are located in the technical

*See Appendix H.

divisions of NBS and in universities, industrial laboratories, and other Government laboratories. Close association between data evaluation projects and relevant experimental research programs helps provide the critical judgment which is essential to assure the reliability of the final output.

The principal output of the program consists of compilations of evaluated data and critical reviews of the status of data in particular technical areas. Evaluation of data implies a careful examination, by an experienced specialist, of all published measurements of the quantity in question, leading to the selection of a recommended value and a statement concerning its accuracy or reliability. The techniques of evaluation depend upon the data in question, but generally include an examination of the method of measurement and the characterization of the materials, a comparison with relevant data on other properties and materials, and a check for consistency with theoretical relationships. Adequate documentation is provided for the selections of recommended values and accuracy estimates.

Evaluated data produced under the NSRDS program are disseminated through the following mechanisms:

Journal of Physical and Chemical Reference Data - A quarterly journal containing data compilations and critical data reviews, published for the National Bureau of Standards by the American Institute of Physics and the American Chemical Society.

NSRDS-NBS Series - A publication series distributed by the Superintendent of Documents, U.S. Government Printing Office.

Appropriate publications of technical societies and commercial publishers.

Magnetic tapes, on-line networks, and other computer-based formats.

Response by OSRD and individual data centers to inquiries for specific data.

PROGRAM STRUCTURE

Current activities in the Standard Reference Data program are carried out in 22 data centers and approximately 32 short-term projects located in the technical divisions of NBS and in academic and industrial laboratories. Each of these activities undertakes the collection and evaluation of the available data on a specified set of properties and substances. The activities are aggregated into three application-oriented program areas:

Energy and Environmental Data - Includes data from fields such as chemical kinetics, spectroscopy, and radiation physics and chemistry which have application to energy-related R & D and environmental monitoring and modeling.

Industrial Process Data - Covers primarily thermodynamic and transport properties of substances important to the chemical and related industries.

Materials Properties Data - Includes structural, electrical, optical, and mechanical properties of solid materials of broad interest.

Since comprehensive coverage of all properties and materials of importance in these three program areas is not feasible, the Office of Standard Reference Data (OSRD) selects data sets of highest priority, based upon the present and anticipated applications of the data. The current focus in each area is described in the sections below.

In addition to its planning and coordinating role, OSRD is responsible for dissemination of the results from the projects that it supports. The principal means of dissemination is still hard-copy publications, although computer-based distribution is becoming more important, as described below. Response to specific inquiries for data directed to OSRD and the individual data centers forms another dissemination mode.

The following tables summarize the published output of the program and the distribution of this output:

Publications in 1982

Series	Pages Published	Titles Published
JPCRD, Vol. 11	2137	22
NSRDS-NBS Series	821	4
Data Compilations in other NBS series	590	6
Data Compilations from other publishers	810	3

Publications in 1982 (cont.)

Series	Pages Published	Titles Published
Bibliographies and indexes in NBS series	55	1
Bibliographies and indexes from other publishers	1380	4
Machine-Readable Data Bases		4
Totals	5793	44

Subscribers to JPCRD

Month/Year	Number
9/1978	1205
9/1979	1237
9/1980	1234
9/1981	1265
9/1982	1234

Inquiries Received in OSRD

(Does not include inquiries received by data centers)

Year	Number
1978	730
1979	882
1980	787
1981	657
1982*	613

Sales of JPCRD Offprints and Supplements

Year	Offprints	Supplements
1978	5577	184
1979	5981	137
1980	5079	111
1981	4254	137
1982*	3567	266

* Projected to end of year

ENERGY AND ENVIRONMENTAL DATA

L. H. Gevantman, Program Manager

The objectives of this program are to contribute to the solution of national energy and environmental problems by providing government and industry with properly evaluated physical and chemical data. These data bases support the more effective use of present energy sources and the development of new sources while helping to protect public health and safety through the improvement of environmental quality.

Effort is directed toward the compilation, evaluation, and dissemination of physical property data on materials that are involved in the production, conservation, and storage of energy. The program impacts such applications as modeling combustion processes for increased energy efficiency, designing improved batteries for energy storage, and developing new materials and systems for use in energy production.

Similarly, the provision of physical property data on environmental pollutant behavior makes an important contribution toward improving air and water quality. These data support industry's efforts to meet clean air and water regulations as well as improve health and safety in chemical manufacturing activities. At the same time, they contribute to government (federal, state, and local) attempts to both regulate and clean up the Nation's environment.

The data required span most of the disciplinary areas embraced by the OSRD but emphasize the fields of kinetics, thermodynamics, and atomic and molecular science. The work of compiling and disseminating these data is performed within 11 data centers supported partially or totally by the OSRD. In addition, a number of grants are awarded for short-term data projects which enlarge the scope of the program.

Activities within the energy program have continued unabated. The series on physical properties data for energy conservation has been completed. High temperature kinetic rate constant data relating to jet and rocket propulsion and prepared in data sheet format will be published in the coming year. Thirty-four elementary reactions are covered.

Progress related to fusion energy continued with the issuance of atomic energy level data on the transition metals. A publication on the energy levels of iron also has been issued. Similarly, the atomic transition probability data on transition metals will be published in the coming year. The newly reorganized data center dealing with photon and charged particle interactions with matter completed its photonuclear program with the publication of the Photonuclear Data Index and is now turning to data on proton interactions. New efforts by the Atomic Collision Cross Section Data Center have resulted in a bibliography on multiphoton interactions.

Four additional manuscripts are in varying stages of completion; the subject matter ranges from electron swarm data to rate coefficients for vibrational energy transfer.

The OSRD project with the Battelle Office of Nuclear Waste Isolation (ONWI) has been concluded with the completion of the basalt data compilation.

The environmental program has also progressed. The selection of evaluated infrared data has advanced the realization of an automated IR data file. Testing of mechanisms for the digitization of these data has been successfully completed. The actual digitization of the data will proceed in the coming year. This effort will be coordinated closely with the NIH and EPA who are providing financial support. The Joint Committee on Atomic and Molecular Physical Data and the Coblentz Society are involved in the conduct of this effort.

Data on solubilities of chemical substances in the environment continue to be accumulated. The solubility of oxygen and ozone in water and seawater will soon be published. Close collaboration continues with Commission V.8 of the International Union of Pure and Applied Chemistry.

Kinetic data relating to atmospheric and stratospheric pollution have also been published. They include rate constants for gas phase reactions of sulfur compounds and data sheets on chemical and photochemical reactions in the stratosphere. A directory of data sources for chemical kinetics was also issued by CODATA in collaboration with the OSRD.

A large effort has been made to convert hard-copy data files to automated form. Many of the data centers are still undergoing such conversions. Those files that have emerged are candidates for on-line dissemination. The infrared data base is to be assembled and entered first. Other data files such as photon absorption data, chemical kinetic rate constants, and atomic energy level data will be considered at some future date.

The trend toward automation of data files has raised some questions by users on data quality, and these are being given serious consideration by OSRD. A workshop was held at NBS on numerical data quality indicators, which addressed the problem of how best to describe the quality of data found in an automated file. A report documenting the workshop's recommendations will be issued soon under the sponsorship of the Chemical Manufacturers Association.

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Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry: Supp. 1, D. L. Baulch, R. A. Cox, P. J. Crutzen, R. F. Hampson, Jr., J. A. Kerr, J. Troe, and R. T. Watson, JPCRD Vol. 11, No. 2.

Molten Salts Data: Diffusion Coefficients in Single and Multi-Component Salt Systems, G. J. Janz and N. P. Bansal, JPCRD Vol. 11, No. 3.

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Molecular Form Factors and Photon Coherent Scattering Cross Sections of Water, L. R. M. Morin, JPCRD Vol. 11, No. 4.

Chemical Kinetic Data Sheets for High-Temperature Chemical Reactions, N. Cohen and K. R. Westburg, JPCRD Vol. 11, No. 4.

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Rate Constants for Reactions of Aliphatic Carbon-Centered Radicals in Aqueous Solution, A. B. Ross and P. Neta, NSRDS-NBS 70.

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Photonuclear Data Index, 1973-1981, E. G. Fuller and H. Gerstenberg, NBSIR 82-2543.

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Biweekly List of Papers on Radiation Chemistry and Photochemistry, A. B. Ross, Vol. 15.

Annual Cumulation of Papers on Radiation Chemistry and Photochemistry, 1981, A. B. Ross, Vol. 14.

INDUSTRIAL PROCESS DATA

H. J. White, Jr., Program Manager

This portion of the overall OSRD program is focused on the needs of industry in developing, designing, and operating plant processes. Major emphasis is placed on the chemical and petrochemical industries.

This is a very active field at the present time. Energy and feedstock costs and supplies are unstable, and mandated safety and pollution controls introduce new constraints. Computer modeling of processes and plants offers new opportunities in a very competitive environment. These have led to the redesign of many old processes and the introduction of many new ones.

Analyses of chemical operations and surveys of industrial scientists and engineers have shown that the properties most frequently needed in process design are the thermodynamic and transport properties of the substances and mixtures being processed. This is reflected in the structure of this program which is primarily composed of projects to produce reference data in these areas.

It is obvious that the activities in the programs on Energy and Environmental Data and Materials Properties will also develop data of importance in industrial process design. The Industrial Process Data program is designed to coordinate with and reinforce these other OSRD programs.

Thermodynamics data can be roughly divided into those that describe chemical reactions and those that describe the behavior of non-reacting substances or mixtures when the temperature, pressure, and--for mixtures--composition are changed. These can be called thermochemical properties and thermophysical properties, respectively, and the program is roughly divided into these two parts. The most frequently needed transport properties are the thermal conductivities of solids and fluids and the viscosities of fluids. The transport properties are classified as thermophysical properties.

Thermochemical properties will be considered first. Since changes in thermodynamic state functions are dependent only on the initial and final states and not on the path between, it is possible and convenient to consider all chemical reactions at one standard temperature and pressure. Auxiliary calculations are used to describe the changes in the reactants and products when going from the desired reaction conditions to the standard conditions.

The task of providing data describing reactions at the standard conditions is covered by the Chemical Thermodynamics Data Center at NBS for inorganic and simple organic substances. Additional work on organic

substances is provided by the Thermodynamics Research Center at Texas A & M. Some specific substances are covered by the JANAF group at Dow Chemical. The Aqueous Electrolyte Data Center works closely with the Chemical Thermodynamics Data Center, providing data needed in describing reactions in solution. These data describing the properties of aqueous electrolyte solutions have a large range of additional uses as well.

The largest portion of the thermophysical properties area is devoted to preparing critically evaluated data on the thermodynamic properties of pure substnaces and their mixtures. Although the majority of industrial process streams are mixtures, the data for pure substances are valuable in their own right and form the base for the prediction and expression of behavior of mixtures.

The program involves two major efforts to provide evaluated data for mixtures, one at the Fluid Mixtures Data Center at NBS Boulder Laboratories and one at the Thermodynamic Research Laboratory at Washington University in St. Louis. The Polar Fluids Data Project at NBS is also working on mixtures. All three projects are concerned with pure fluids as well.

The transport properties of solids and fluids are being evaluated by the Center for Numerical Data Analysis and Synthesis (CINDAS) at Purdue University. Further work on the transport properties of fluids is being carried out at the Fluid Mixtures Data Center in Boulder and at Brown University. An international group under IUPAC sponsorship is also focused around the activities at Brown.

This is a period of transition for several of the major data activities in the Industrial Process area. Five major monographs have been or will be published within a six- to nine-month period. Completion of these major tasks will free resources and people for other activities.

It is also worth noting that four of the five monographs were submitted in fully automated form as were the tables for the fifth. Furthermore, the tables from one are already available on the Chemical Information System (CIS), an interactive computer network. The center which has produced one of the others is already entering data on CIS in an experimental mode. It is probable that some of the contents of this second monograph will be available on CIS in due time. Companion publications for two of the others contain instructions for mounting the reference data involved on the user's own computer. From this it is apparent that the four data centers from which these monographs come are strongly involved in computerizing their operations and that they and OSRD are producing computer products as well as conventional books.

Another trend, which is assisted by the drive toward automation, is increasing participation in cooperative activities. The possibility of making more efficient and effective use of limited resources through cooperative projects is a strong stimulus. The CODATA Task Group on

Internationalization and Systematization of Thermodynamic Tables (CODATA ISTT) has recently completed a systems analysis of the preparation of thermodynamic tables and, on the basis of this analysis, has submitted a plan to CODATA for an automated, decentralized, international system for producing thermochemical tables. Representatives of several OSRD activities participated in the systems analysis and planning, and three data centers are reconfiguring themselves in response to it.

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Heating Values of Natural Gas and Its Components, G. T. Armstrong and T. L. Jobe, Jr., NBSIR 82-2401.

A Compilation of Thermodynamic and Transport Properties of Aqueous Potassium Hydroxide, R. E. Joseph and B. R. Staples, NBSIR 81-2356.

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Bulletin of Chemical Thermodynamics, R. D. Freeman, Ed., Vol. 24, Oklahoma State University Press, Stillwater, Oklahoma.

MATERIALS PROPERTIES DATA

J. R. Rumble, Jr., Program Manager

The Materials Properties Data Program has been designed to provide evaluated materials property data to the U.S. materials industry and materials researchers. The program presently concentrates on several areas--phase stability information, crystallographic data, diffusion, mechanical properties, and polymer properties data--and has profited by a number of close-working agreements with various industrial groups.

Phase Stability Information

Phase stability information is basic to a better understanding of materials and their properties and is needed to develop and design new alloys, ceramics, and metallic/nonmetallic systems. OSRD supports two data centers, the Alloy Phase Diagram Data Center and the Phase Diagrams for Ceramists Data Center, which have become the prime source of evaluated phase information in the United States. The centers also have developed strong industrial ties, the Alloy Center with the American Society for Metals (ASM) and the Ceramics Center with the American Ceramics Society (ACerS), which ensures that the output is geared to users' needs.

The Alloy Phase Diagram Center is the focal point of the NBS/ASM joint program to evaluate all alloy phase diagrams. Over the last year, the Alloy Center has exerted vigorous technical leadership of the program, especially with respect to setting evaluation standards, developing new and innovative computer graphics for phase diagrams, and editing the Bulletin of Alloy Phase Diagrams.

The Alloy Center, with support of the Office of Naval Research, has been evaluating phase stability data and phase diagrams for all titanium binary alloy systems. Titanium alloys are of major interest for their light weight, high strength, and other properties. A major part of the evaluation has been to extend a thermodynamic optimization computer program so that it can be used interactively and linked to a computer graphics program. Over 20 titanium systems have been evaluated thus far. In addition to its own merit, the resulting report has been widely circulated to other evaluators as a standard both for quality and format.

Moreover, the Center has begun work on two systems, iron and aluminum, which are of major economic and technical importance. The aluminum work is sponsored in part by the Defense Advanced Research Projects Agency. The evaluation procedure is similar to that for titanium. Several evaluations have been published.

Working closely with the Alloy Center, the NBS Center for Applied Mathematics has developed the computer graphics programs mentioned above. First and foremost, the programs can produce publication quality phase diagrams and now generate the diagrams in the Bulletin of Alloy Phase Diagrams. Both binary and ternary systems can be handled. Initial steps have been taken to develop a computer database for phase information. The database will include a graphic and functional representation of the phase diagram data, text, and thermodynamic, crystallographic, and bibliographic data in a searchable computer file. This aspect of the work will be done with the help of ASM research associates working at NBS.

The Bulletin of Alloy Phase Diagrams, now in its second year of publication, has quickly become a major source of evaluated phase information. Full technical responsibility resides with the Alloy Data Center. The ASM has the publishing responsibility.

In addition, OSRD supports several other phase data evaluation projects via the OSRD grants programs. The binary systems now covered include copper, vanadium, niobium, the alkali metals, and the rare earths. Many evaluations of these systems have been already published in the Bulletin. OSRD also interacts with the International Council on Phase Diagrams and works with that group and ASM to find other evaluators and to ensure all evaluations are of high quality. As the number of evaluated systems grows, monographs will be published and the data made available to the computer database.

Ceramics phase diagrams have taken on new importance in recent years as the ceramics industry has grown into innovative areas such as ceramics for high-strength and high-temperature application and metals bonded on ceramic-base materials.

In a joint effort with the American Ceramics Society, the Phase Diagrams for Ceramists (PDFC) Data Center has for many years been involved in the evaluation of ceramics phase diagrams. The fifth volume in the Phase Diagrams for Ceramists Series was completed recently and will be published shortly.

The data center and the ACerS are now exploring ways to strengthen the program and meet the increasing demand for more evaluations on more systems. The two major aspects of the proposed enhanced program are to increase support for evaluation and to build a ceramics phase diagrams database. To be able to provide more evaluations each year, the PDFC and the ACerS hope to increase the support for evaluation so that significantly more work can be done. This would also greatly increase the frequency of publication of volumes in the Phase Diagrams for Ceramists Series. Discussions are presently under way to involve the ceramics industry more closely in this program, and in the upcoming year it is hoped that key support will be forthcoming.

OSRD has been working closely with the PDFC Center to develop a bibliographic database for both their use and that of other data centers using the NBS central computing facilities. The design stage has been completed, and OSRD has started the programming.

The PDFC phase diagram database is at a much less mature state than the alloy database. However, much of the experience gained by the Alloy Center will be directly applicable to the PDFC effort. Both the design and the programming stages should be greatly shortened by the sharing of experience, a process in which OSRD will be heavily involved.

Crystallographic Data

Crystallographic data activities have in recent years reached a very high level of sophistication, which reflects the maturity of the science, the early use of computers by crystallographers, and the growing importance of such data as an identification tool. OSRD-sponsored activities, including the NBS Crystal Data Center, have played an important role in this process, and in the past year several significant milestones were achieved.

The major event has been the conclusion of a joint agreement with the JCPDS-International Centre for Diffraction Data (JCPDS). This agreement covers two important areas--the dissemination of output from the NBS Crystal Data Center and the building of the data center's master file and other related files. The JCPDS will continue to publish the series "NBS Crystal Data Determinative Tables" and will begin to market the NBS Crystal Data Identification File. Revenue from these products will be used to support abstracting services and database building and maintenance to ensure current coverage.

The other significant event has been the release of the NBS Crystal Data Identification File by the NBS Crystal Data Center. This file has been installed as part of the NIH/EPA Chemical Information System (CIS) and is available for on-line computer use. The file contains crystallochemical information on over 60,000 materials and is of great use both as an analytical tool and as a means of determining what crystallographic work exists for a given species.

In addition to the NBS data center, OSRD has supported several other worldwide crystallographic projects which interact strongly with the NBS center. The on-going contract with the Cambridge Crystallographic Centre has this year centered on providing the organic entries to the Crystal Data Identification File. The other major effort has been to process the Cambridge file through NBS*AIDS80 and create master file entries for the organic substances. This output will be used in the coming year to publish two more volumes in the Crystal Data Series which will contain new data on 20,000 organic substances.

Also, an agreement was reached with the crystallographic group at the University of Bonn, West Germany, to provide data for inorganic materials on which full structural determinations have been done.

Diffusion Data

Diffusion in metals has two major areas of interest in the metals industry: performance and new materials. Diffusion of impurity or alloying constituents plays an important role in determining the performance and useful life of materials in actual use. In recent years, diffusion has also become an important method of altering the surface characteristics of materials, especially to provide high performance properties to a less costly base metal.

The Diffusion in Metals Data Center has been active in providing evaluated diffusion data to the industrial community and others.

The Center has finished work on the evaluation of data relating to mass transport and diffusion phenomena in the durability of copper and its alloys, especially multicomponent alloys. These systems are of great interest with respect to understanding and avoiding corrosion problems. This work has been sponsored in part by the International Copper Research Association (INCRA) and has been published this year as Volume 8 of their series on the metallurgy of copper.

Additionally, the Data Center has continued an automation project which will greatly facilitate their close interaction with the industrial community as the primary source of data in all alloy diffusion areas.

Mechanical Properties

Mechanical Properties are an important class of data fundamental to the design, manufacturing, and performance of most engineering materials. Most such information has been compiled, evaluated (infrequently), and distributed by materials producers, technical societies such as ASTM, ASME, and MPC, data centers, and technical publishers. In recent years there has been some movement towards creating comprehensive materials information databases; such efforts would require the cooperation of several interested groups.

During the past year, OSRD has been involved in two activities bearing on this subject. First, we helped support the Metals Properties Council's feasibility study on intersociety materials databases. This study examined various issues associated with creating large databases, and its final report will be available late this year.

Also, OSRD has helped sponsor the Materials Data Workshop, which is to be held November 7-11, 1982. At the workshop, representatives from all groups interested in this subject will participate in intensive discussions of the many issues relating to it. The results of the workshop are expected to shed light on the best way to proceed.

Polymer Properties

A small project on Polymer Solution Viscosity Data has been started in the Polymers Division at NBS. This effort will compile and critically assess viscosity data relating to molecular weight parameters for polymers in various solvents. The systems to be studied include important polymers such as polyethylene and polystyrene.

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J. L. Murray, BAPD 2.

Tc-Ti System
J. L. Murray, BAPD 2.

Al-Mg System
J. L. Murray, BAPD 3.

Al-Li System
A. J. McAlister, BAPD 3.

Al-Be System
D. J. Kahan, BAPD 3.

Al-Zn System
J. L. Murray, BAPD 3.

Al-Cd System
A. J. McAlister, BAPD 3.

Al-Ga System
M. E. Read, BAPD 3.

Al-In System
D. J. Kahan, BAPD 3.

NBS Crystal Data Identification File. Available via the NIH/EPA Chemical Information System and the JCPDS-International Centre for Diffraction Data.

AUTOMATION

J. R. Rumble, Jr., Program Manager

The growth of technology and increase in the availability of computers have given rise to a demand for data dissemination by computer-based methods. This demand has coupled with a need for more efficient and less costly data center operations to produce a major commitment by the Office of Standard Reference Data to automate the internal operations of its data centers and to develop machine-readable numerical databases for on-line dissemination.

The major highlights of this year's activity include releasing two databases for public use on a computer network and obtaining necessary computer facilities for automation of several data centers. Also, the deep commitment by OSRD and its data centers continues.

On-Line Data Bases

Two major NBS databases have been released for public use on the Chemical Information System (CIS). These are the NBS Crystal Data Identification File and the NBS Chemical Thermodynamics Database. Both of these files resulted from the combination of ongoing data center activities with a special effort to answer the need for machine-readable data in these areas.

The databases are accessible to the public through a computer which can be reached by telephone. The databases have been supplemented by software written under contract for OSRD. This software allows the user to search the file and use the data in a meaningful way. In addition, the full power of the CIS is available. These databases represent the first two of what will be a long series of NBS/OSRD machine-readable databases.

NBS Computing Facilities

The NBS Central Computing Facility (CCF) this year upgraded their hardware to a UNIVAC 1100/82 mainframe. In addition to this, the CCF completed plans for procuring a computerized typography system which will be heavily used by OSRD's Data Systems Development Group in producing quality data publications. The new system is expected to arrive in mid-1983.

To supplement the CCF and to take care of specific data center needs, OSRD has purchased a Hewlett-Packard 1000 minicomputer. Several data centers will use this machine for data entry and data base building.

Other Data Base Activities

Design and programming work has continued on many databases associated with OSRD data activities which are listed in table I and, in the next 18 months, we anticipate that two or more additional databases will be released for public use.

In addition to database efforts created within OSRD's data centers, OSRD has played a major supportive role with groups interested in materials data and chemical process data. OSRD has also continued to work with the CIS on maintaining their on-line system.

Table I

OSRD Activities in Numerical Data Bases

Crystal Data
- NBS Crystal Data Identification File
- NBS Master Crystal Data File (with Cambridge, Bonn, Ottawa)

Chemical Thermodynamics
- Inorganic Compounds - NBS
- Organic Compounds - Texas A & M
- Temperature-Dependent Inorganic (JANAF) - Dow Chemical

Phase Diagrams
- Alloy (with ASM)
- Ceramics (with ACerS)

Atomic Spectra
- Energy Levels
- Transition Probabilities

Kinetics of Chemical Reactions
- Combustion Reactions
- Atmospheric Reactions
- Photo-initiated (Fast)

Properties of Fluid Mixtures
- Hydrocarbons
- Polar Molecules

Collision Cross-Section
- Electrons
- Photon and Charged Particles

DATA CENTER AND PROJECT REPORTS

The following pages provide brief descriptions of the scope and activities of each of the continuing data centers and short-term projects within which the data evaluation and compilation work is carried out. The data centers are listed in alphabetical order by name, The short-term projects are categorized by the OSRD program area under which they are managed.

ALLOY PHASE DIAGRAM DATA CENTER

Kirit Bhansali, Director
Center for Materials Science, NBS

The Alloy Phase Diagram Data Center collects, evaluates, and distributes phase stability data for metal alloy systems and is the technical coordinator for the NBS-ASM Alloy Phase Diagram Program.

The Center is responsible for the technical content and editing of the Bulletin of Alloy Phase Diagrams, a joint publication with the American Society of Metals. The Bulletin has rapidly become the prime source of evaluated phase data. Computer graphics software for phase diagrams has been developed and is used to help produce the Bulletin.

A vigorous evaluation program for titanium systems, with support by ONR, is now well in its third year, and more than 20 titanium binary systems have been evaluated. Evaluation of aluminum systems has begun, and seven aluminum binary systems have been completed. This work is supported in part by DARPA. In addition, work on iron systems has started. During this evaluation effort, thermodynamic optimization programs have been enhanced and interfaced with the graphics software.

Preliminary work for designing and creating a data base of phase information and ancillary data has been completed. This was done in close cooperation with the ASM.

AQUEOUS ELECTROLYTE DATA CENTER

Bert R. Staples, Director
Center for Chemical Physics, NBS

The Center provides the chemical process and related industries with critically evaluated data on the thermodynamic properties of aqueous electrolyte solutions including activity and osmotic coefficients, excess and partial molar properties of solution, solubilities, and equilibrium constants in solution. It also provides information services and techniques for correlation and estimation of such properties.

The Center is closely coordinated with the Chemical Thermodynamics Data Center, using its bibliographic resources and providing it with evaluated data on aqueous systems as needed.

Projects recently completed or nearing completion are described below:

Heat capacity and enthalpy of dilution data have been correlated for aqueous $CaCl_2$ solutions. These results have been employed in tables of

thermodynamic properties being prepared by CODATA ISTT.

Correlations of activity coefficients as a function of concentration have been prepared for 197 aqueous electrolytes using the Pitzer equations as a model. The Pitzer equations are an effective form of semi-theoretical correlating equations for activity data. These are finding wide applications in chemistry and in chemical engineering. These evaluated data will be made available as a data base calculation program package.

Recommended values have been prepared for the solubility of gypsum, $CaSO_4.2H_2O$, as a function of temperature and added salt concentration. It has been shown in this work that the theoretical treatment of salt mixtures developed by Pitzer reproduces the experimental data very well and, in this case, is better than other approaches. This work has been done to provide evaluated data and calculational example for a handbook being prepared by the Design Institute for Physical Property Data (AIChE). It is also pertinent for coal/flue gas cleanup systems.

Heat capacity data have been compiled and correlated for aqueous solutions of S(IV) and S(VI) compounds of Fe, Ni, Mn, Na, K, Mg and Ca. These data are needed for extending the temperature range of recommended data for enthalpies of dilution and activity coefficients. The substances were chosen because of their occurrence in coal/flue gas cleanup systems.

The Center is currently involved in developing a procedure for the calculation of the vapor-liquid equilibrium composition of solutions of weak, volatile compounds such as the system $SO_2 + H_2O$ and the equilibrium vapor phases. The procedure involves an intricate, self-consistent calculation involving equilibria both in the gas phase and in solution.

Also under development is a more general procedure which can be used to calculate the excess and partial molar properties of aqueous electrolyte and non-electrolyte solutions which associate, hydrate, or hydrolyze.

ATOMIC COLLISION CROSS SECTION DATA CENTER

Jean W. Gallagher, Director
Center for Absolute Physical Quantities, NBS

The Center's aim is to compile, evaluate, and disseminate data concerning electron and photon collisions with atoms, simple molecules, ions, and low energy heavy particles. Emphasis is given to electron-collisional excitation and ionization, heavy particle energy transfer, photoionization, photodetachment, and photofragmentation.

With the appointment of a permanent director to the data center the pace of activity at the center has increased. In the past year five manuscripts have been submitted for publication. They include a multi-photon ionization data bibliography as well as data compilations on such

subjects as cross sections for electron scattering and ion-atom charge exchange, electron swarm data, and rate coefficients for vibrational energy transfer involving the hydrogen halides. Work has also continued on the automation of the data center files through the procurement of a microcomputer.

New data projects are planned for the coming year. They include the compilation of data on energy transfer in diatomic halogens, proton impact ionization phenomena, elastic scattering in alkalis and mercury vapor, electron affinity, and electron excitation of ions of astrophysical interest. The data management system should also be completed thereby improving the data center's operation.

ATOMIC ENERGY LEVELS DATA CENTER

W. C. Martin, Director
Center for Radiation Research, NBS

The Center compiles, evaluates, and disseminates data on energy levels and spectral lines of atoms and atomic ions. Reliable atomic spectroscopic data are essential to the interpretation of measurements in such areas as plasma diagnostics and astronomy.

The compilation of the fourteen spectra of the astrophysically important element silicon were completed this year. Work was also completed and published on the energy levels of iron and cobalt. Preliminary work on phosphorus and sulfur spectra has begun.

Considerable progress has been made on updating the iron-group compilations for collection into a single volume for all 235 spectra of these ten elements (K-Ni). Additions and corrections were also made to the tables of wavelengths published in the CRC Handbook of Chemistry and Physics.

Future effort will be devoted to completion of the cumulative iron-group compilation. Results of previous work will enable a more direct and critical evaluation of the new data by working along isoelectronic sequences. It is also expected that new compilations will be completed for the most important spectra in the element group phosphorus through argon.

Close collaboration with the Atomic Transition Probabilities Data Center will be maintained.

ATOMIC TRANSITION PROBABILITIES DATA CENTER

Wolfgang L. Wiese, Director
Center for Radiation Research, NBS

The Center's purpose is to compile, evaluate, and disseminate data on atomic transition probabilities and lifetimes of excited levels of atoms and atomic ions. Interpretation of fusion plasma diagnostic techniques is highly dependent on the availability of these data.

Effort continues on the preparation of atomic transition probability data tables for the allowed and forbidden lines of the elements scandium through nickel. Data for the allowed lines are being completed and work is starting to evaluate the forbidden line data. The recommendations contained in an exploratory review of the data center's requirements for an automated system are being implemented. Close attention is being given to the relationship between this Center's requirements and those of the Atomic Energy Level Data Center.

Future plans call for the completion of the iron group elements data. Some work will be initiated on transition probability data for selected heavy elements (zirconium, etc.). Finally, continued effort will go into the completion of an automated data file.

CINDAS (Center for Information and Numerical Data Analysis and Synthesis)

C. Y. Ho, Director
Purdue University
West Lafayette, Indiana

This is a large data center which receives support from a number of sources. It compiles and evaluates data on transport properties, heat capacities, thermal expansion, and optical, electronic, and electrical properties for a wide range of substances. For OSRD, CINDAS has been involved in the compilation and evaluation of data on thermal conductivity and electrical resistivity of metals and alloys and the thermal conductivity, viscosity, and heat capacities of fluids.

A monograph on the electrical resistivities of a set of binary alloys is in press. A monograph on the thermal conductivities of the same alloys has already been published and a report on the thermoelectric power of the same alloys is nearing completion.

The second of a three part series of publications on the viscosity, thermal conductivity and heat capacity of a set of seventy-six fluids of industrial importance is nearing completion. It will contain data on 29 substances. The first volume has been published and the third is in preparation.

CHEMICAL KINETICS DATA CENTER

R. F. Hampson, Director
Center for Chemical Physics, NBS

The Center compiles, evaluates, and disseminates chemical kinetic data in support of industrial productivity and environmental integrity. It also develops models and algorithms for the extension and prediction of kinetic parameters.

Publications issued this year included a bibliography on sulfite ion oxidation in solution, rate constants for gas phase sulfur compound reactions and a compilation of experimental rate constants on combustion reactions. The CODATA Task Group report on stratospheric chemistry has also been completed and will be published soon. The Chemical Kinetics Data Center made major contributions to this report, and the head of the Center serves as Secretary of the Task Group. Work has begun on automating the numerical data file within the Center.

Future activities will be directed toward automated data management and the compilation and evaluation of rate data for reactions related to atmospheric chemistry and to combustion.

CHEMICAL THERMODYNAMICS DATA CENTER

David Garvin, Director
Center for Chemical Physics, NBS

The Center provides the chemical process and related industries with critically evaluated thermodynamically compatible data which can be used to establish the equilibrium constants and heats of reaction for important chemical reactions. It provides data describing the change in the chemical properties of substances with changes in temperature and at phase-transition points, as well as bibliographic reference services on thermochemistry. In particular, the Center provides enthalpies and Gibbs energies of formation, entropies and Cp in the standard state at 298.15 K and 1 atm.; enthalpies of formation at 0 K for inorganic substances and simple organic substances; transition properties; and thermal functions.

A major task completed this year is the publication of "The NBS Tables of Chemical Thermodynamic Properties" providing 26,000 data items on 14,500 substances. These tables are in SI units and use a pressure base of 0.1MPa rather than 1 atmosphere. The tables are corrected and contain updated values for some 450 gaseous ions. The data in the tables are also available on the CIS interactive network. Other tasks completed during the year involve new evaluations of selected compounds of calcium, the uranium halides, and C_1 and C_6 aliphatic hydrocarbons. Each of the latter tasks has international implications. The first provides part of a set of tables prepared by CODATA ISTT. Other parts have been prepared

by the JANAF group and by groups in France, the UK and the USSR. The tables on the uranium halides are part of a set of tables being prepared by the International Atomic Energy Agency. The hydrocarbon data were prepared under the sponsorship of the International Group of Importers of Liquified Natural Gas (GIIGNL).

The Center prepared the Inorganic Section of the Bulletin of Chemical Thermodynamics, which contains material from 4,128 references, as well as the index to the entire Bulletin. The Bulletin is published annualy.

Current major efforts involve preparation of reaction catalogs and automation of various steps in the process of preparing tables. Reaction catalogs are machine readable (and man readable) listings of measurements. They serve two purposes. They are input to network-solution programs which assist evaluators in introducing thermodynamic consistency into tables, and serve as documentation to the tables prepared. Total or partial reaction catalogs exist for some 20 odd elements.

CRYSTAL DATA CENTER

A. D. Mighell, Director
Center for Materials Science, NBS

The Crystal Data Center is concerned with crystallographic data that are required for the identification and characterization of solid state materials. To facilitate the collection, evaluation, and dissemination of these data, a master Crystal Data File is being created, and a fully automated data center will be based on this file.

The Crystal Data Center has recently concluded a comprehensive agreement with the JCPDS-International Centre for Diffraction Data. The agreement provides for the distribution of the NBS Crystal Data Determinative Tables series and the NBS Crystal Data Identification File by the JCPDS-ICDD. In addition, the agreement allows for an increased effort to build and maintain the NBS Crystal Data Center master file and outputs from it.

The NBS Crystal Data Identification File with data on about 60,000 materials and a computer program for the evaluation of crystallographic data have been released to the crystallographic community. The Crystal Data Identification File also is distributed by the on-line NIH/EPA Chemical Information System. It is updated yearly with new data obtained from the literature and from allied data centers in England, West Germany, and Canada.

During the coming year, the Crystal Data Center will concentrate on publishing the next two volumes in the NBS Crystal Data Determinative Tables series. These will contain data on over 20,000 new organic materials supplied by the Cambridge Crystallographic Centre. The NBS Center will also be working on search software for the Crystal Data Identification File.

DIFFUSION IN METALS DATA CENTER

John Manning, Director
Center for Materials Science, NBS

The Diffusion in Metals Data Center is concerned with data on diffusion rates and mass transport in metals and their alloys.

The Center has recently completed a second volume of critically evaluated data dealing with diffusion in copper alloy systems. This work was done under a cooperative agreement with the International Copper Research Association (INCRA) and is published as part of the INCRA series on the Metallurgy of Copper. It will be a companion to an earlier volume concerned with a different group of copper alloys. The next evaluation project will be concerned with diffusion in iron-chromium systems.

The data center is in the midst of an intensive effort to automate. The large data base on diffusion literature is being entered onto an on-line system, which will allow maintenance, updating, and retrieval of the information as needed. Specialized bibliographies on selected diffusion will be prepared as the data are entered into the system.

FLUID MIXTURES DATA CENTER

Neil Olien, Director
Center for Chemical Engineering, NBS

The Center is organized to compile and evaluate data on the thermodynamic and transport properties of fluids and fluid mixtures. These properties include formulations for the density and other thermodynamic properties of pure fluids, the viscosity and thermal conductivity of pure fluids, and the same properties for fluid mixtures. The Center is also involved with the development of techniques to predict transport properties of pure fluids from thermodynamic and molecular data, to predict properties of mixtures from the properties of pure fluids, and to interpolate and extrapolate data for properties over a range of temperature, pressure, and--in the case of mixtures--relative concentrations.

A major task recently completed was the publication of a table containing the thermodynamic and transport properties of six fluids. The same set of equations was used for each fluid so that properties for the various fluids are obtained by using different sets of coefficients as input. A companion publication which provides software for the use of the equations has also been prepared. Tables for a second set of fluids are in preparation.

A computer program called TRAPP which predicts thermodynamic and transport-property data for mixtures of fluids has also been made available. Considerable effort is being made also to extend and improve this program.

FUNDAMENTAL CONSTANTS DATA CENTER

Barry N. Taylor, Director
Center for Absolute Physical Quantities, NBS

The Center provides a centralized source of information on the fundamental physical constants and on closely related precision measurements. The Center participates in the periodic development of sets of "best" or recommended values of the fundamental physical constants by means of least-squares adjustments. The self-consistent best values of the constants resulting from an adjustment are required for computational purposes and often are the basis for other data compilations.

A volume was published on the analysis of fundamental constants entitled, "Numerical Comparisons of Several Algorithms for Treating Inconsistent Data in a Least-Squares Adjustment of the Fundamental Constants" (NBSIR 81-2426). The 1982 Least-Squares Adjustment of the Fundamental Constants should be completed and published in early 1983.

ION ENERGETICS DATA CENTER

Sharon G. Lias, Director
Center for Chemical Physics, NBS

The Data Center collects and maintains an up-to-date file of experimental data on the thermochemistry of ions (ionization potentials, appearance potentials, and equilibrium constants) and the kinetics of ion molecule reactions. Evaluated compilations of this data are disseminated to the scientific and technological community.

A compilation of all the ionization potential and appearance potential measurements appearing in the literature from 1971 through March, 1981, has been completed. Including approximately 20,000 data items, the compilation was edited and re-formatted into a shorter, more readable form than the previous publication. The book should appear shortly.

A preliminary evaluation of the heats of formation of 200 ions in the gas phase was carried out for the Chemical Thermodynamics Data Center and is being published as an appendix to the NBS Thermochemical Tables. The evaluation involved the efforts of three NBS senior scientists, as well as experts from the University of California, Indiana University, the University of Maryland, and the University of Ottawa.

A future volume will present evaluated proton affinity data. These data will be related to the corresponding liquid phase basicities, and an analysis will be presented of the kinetic and thermochemical differences between gas and liquid phase proton transfer reactions, especially in those biochemical systems for which gas phase data are available.

JANAF THERMOCHEMICAL TABLES

Malcolm W. Chase, Jr., Director
Dow Chemical Company
Midland, Michigan

The JANAF Thermochemical Tables Center covers the thermodynamic properties for the crystal, liquid, and ideal gas state over a wide temperature range. Properties covered are heat capacity, entropy, Gibbs energy function, enthalpy, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound from the elements in their standard reference states.

Published tabulations involve 35 elements and their compounds. The 35 elements are H, Li, Be, B, C, N, O, F, Na, Mg, Al, Si, P, S, Cl, K, Ca, Ti, V, Cr, Fe, Co, Cu, Br, Sr, Zr, Nb, Mo, I, Cs, Ba, Ta, W, Hg, and Pb.

The Center also generates specified tables of thermodynamic properties, literature surveys, and various automated outputs, largely in connection with the development of an international system for producing chemical thermodynamic data.

A supplement to the existing tables was published by the Center this year. The Center is also involved in the preparation of a complete revision and updating of its published tables. The Center has also been active in the work of CODATA ISTT.

MOLECULAR SPECTRA DATA CENTER

Frank J. Lovas, Director
Center for Chemical Physics, NBS

The Center provides for the collection, evaluation, and dissemination of molecular spectral frequencies and other molecular constants. These are designed to aid in the analysis and identification of compounds and to permit assignment of a wide range of molecular properties. One phase of the Center's work emphasizes microwave spectra of interstellar molecules.

Two publications have been issued; one on N_2O absorption lines for tunable laser calibration in the infrared and the other on microwave spectra of ethanol and propionitrile. Some effort has been expended on producing a microwave spectral line data tape of known interstellar molecules.

In the future, effort will be given to completing the microwave spectral line data tape. A publication on C_2H_2 standard frequencies in the infrared is also planned.

MOLTEN SALTS DATA CENTER

George J. Janz, Director
Rensselaer Polytechnic Institute
Troy, New York

The Center's goals are to compile, evaluate, and disseminate physical properties data on selected molten salts.

Activities of the Center have produced a document on evaluated diffusion coefficient data in single and mixed component molten salt systems. This document is now in press. In addition, another document on other molten salt properties and systems is nearing completion. The Center is introducing an automated data management system and has converted its bibliographic file from manual to automated form.

Future activities will include the accumulation of the molten salt data into an updated single volume. In addition, automated tape files of numerical data will be produced starting with molten salt eutectic data.

NATIONAL CENTER FOR THE THERMODYNAMIC DATA OF MINERALS

John L. Haas, Jr., Director
U.S. Geological Survey
Reston, Virginia

The Center compiles, indexes, and evaluates data on the thermodynamic and thermophysical properties of minerals, their synthetic analogs, and geologic materials. These data are important for geochemical purposes and useful industrially in the fields of metallurgy and the synthesis and production of inorganic chemicals.

In particular, the Center develops critically evaluated thermodynamic data for naturally occurring solid phases or their chemical end members. Properties considered are heat capacity, entropy, enthalpy, Gibbs energy, enthalpy and Gibbs energy of formation, molar volume, molar compressibility, and molar expansivity, all as functions of temperature, and phase diagrams of systems containing mineral phases. The Center cooperates closely with the Chemical Thermodynamics Data Center and the JANAF Thermochemical Tables Project.

Some recent activities have centered about properties of geologic structures suggested as burial sites for high-level nulcear wastes.

PHASE DIAGRAMS FOR CERAMISTS DATA CENTER

L. P. Cook, Director
Center for Materials Science, NBS

The Phase Diagrams for Ceramists (PDFC) Data Center has two primary goals: the regular publication of evaluated phase stability information for inorganic nonmetallic systems and the development of a computer-searchable "Phase Diagrams for Ceramists" data base.

The PDFC Center has published jointly with the American Ceramic Society the series "Phase Diagrams for Ceramists." Volume 5 will contain 650 diagrams of molten salts, sulfides, oxynitride systems; work on this volume has substantially been completed. It is scheduled to be published next year. Evaluation work for Volumes 6 and 7 has started.

A comprehensive long-range plan for development of the "Phase Diagrams for Ceramists" data base, in collaboration with the American Ceramic Society, has been developed. The main features of the plan are increased automation involving all aspects of the project and increased evaluation effort. The Ceramic Society has set up the "Ad hoc Advisory Committee of the Phase Equilibrium Data Center" to implement this plan and to begin developing increased industrial support.

The first steps toward the designing and building of a data base have been taken. With OSRD's help, the Center has completed the logical design of its bibliographic data base, and programming will being shortly. In addition, prototype graphics software has been developed, and discussions with the Alloy Phase Diagram Data Center are continuing with respect to mutual problems. As resources allow, the graphics package will be implemented on the OSRD HP 1000 computer.

PHOTON AND CHARGED PARTICLE DATA CENTER

M. J. Berger, Director
Center for Radiation Research, NBS

The Center compiles, evaluates, and disseminates data on the interaction of ionizing radiation with matter. The data on photons and charged particles include single-scattering cross sections and transport data pertaining to penetration of radiation through bulk matter.

The Center's effort has been devoted to converting the photon cross section file from manual to automated format, producing the Photonuclear Data Index, and planning new data compilations for proton and other charged particle interactions with matter.

Future efforts will be directed to preparing tables of proton stopping powers and ranges at energies from 10 keV to 1000 MeV for approximately 50 elements and compounds. The automated management system for photon cross section data will also be improved.

RADIATION CHEMISTRY DATA CENTER

Alberta B. Ross, Director
Radiation Laboratory, University of Notre Dame
Notre Dame, Indiana

The Center's purpose is to compile, evaluate, and disseminate rate parameters and related data on chemical reactions initiated by the interaction of ionizing and photon radiation with matter. Emphasis is placed on those reactions occurring in aqueous and liquid media. Support of the Center is shared by OSRD and the DOE Office of Basic Energy Sciences.

The Center continues to publish the Biweekly List of Papers on Radiation Chemistry and Photochemistry and the Annual Cumulation of the Biweekly List. The number of subscribers continues to grow reflecting the value of this output to the user public. A compilation of evaluated rate constants in singlet state oxygen in solution was published. Work also went into automating the data file within the Center.

Future effort will be directed toward continued publication of the Biweekly List, a publication on evaluated rate constants on aliphatic carbon centered radical reactions in solution, and the continued improvement in the Center's data management system.

THERMODYNAMIC RESEARCH CENTER

K. R. Hall, Director
Texas A&M University
College Station, Texas

The Center provides the chemical process and related industries with critically evaluated data on a wide variety of thermodynamic and thermophysical properties of organic compounds. These include thermodynamic properties of organic materials, condensed-phase properties, transition points and properties, density and vapor pressure of liquids, and ideal gas and real gas properties.

The current principal project of this Center involves the thermochemical properties of compounds containing C, H and O in the C_1 - C_4 range. There are 94 such compounds for which there are calorimetric data, of these there are enough data for a 3rd Law entropy for 36 and suitable data to prepare a reasonable ideal-gas thermal function for 27. The intent of the project is to utilize these resources to obtain as many thermodynamically consistent data as possible on the thermochemistry of this important class of compounds. The work on the condensed-phase properties (3rd Law) and ideal-gas thermal functions has been finished and is in preparation for publication.

The Center is also entering data on the Chemical Information System in an experimental mode and was instrumetal in developing the thermo-

dynamic software used in CIS.

The Organic Section of the Bulletin of Chemical Thermodynamics is prepared by this Center every year.

THERMODYNAMIC RESEARCH LABORATORY

Buford D. Smith, Director
Washington University
St. Louis, Missouri

This laboratory compiles and evaluates data on the vapor-liquid equilibrium, excess enthalpy, and excess volume of binary subcritical fluid mixtures and data on the vapor pressures, enthalpies of vaporization, saturated-liquid densities, and virial coefficients of pure fluids which are components of the mixtures. The laboratory is funded jointly by industry and the Office of Standard Reference Data (OSRD). It covers a wide range of fluid mixtures, but its work for OSRD is focused on hydrocarbon-hydrocarbon systems with carbon numbers C_2 - C_8 and mixtures of hydrocarbons with aliphatic alcohols.

Reports on the excess volume, excess enthalpy and PTxy data for the system, benzene-cyclohexane and benzene-hexane are in press. A similar report on the hexane cyclohexane system is in preparation, as is a report on the remainder of the C_6 - C_6 systems for which there are data.

Work will start shortly on the C_6 and C_7 hydrocarbon systems and on systems containing a hydrocarbon and an aliphatic alcohol.

The Center expects to make these data available on an interactive computer system as well as in report form.

CRITICAL COMPILATION OF MASS SPECTRAL DATA

Martin G. Robiette
Mass Spectral Data Centre
Nottingham, England
Source of Support: NBS

The project compiles, evaluates, and enters mass spectral data into the Chemical Information System (CIS). The data are collected from the open literature and other sources, private and public. Their quality is assessed through the application of a quality index algorithm. Those data that are considered of high quality are submitted for entry into the CIS and are also reproduced in hard-copy form through supplements to NSRDS-NBS 63, the NIH-EPA Mass Spectral Data Base. Approximately 1200-1500 spectra are collected annually.

CRITICAL EVALUATION OF HIGH TEMPERATURE KINETIC DATA

N. Cohen
Aerospace Corporation
Los Angeles, California
Source of Support: DOD and NBS

This project compiles and disseminates evaluated data sheets describing the high-temperature kinetics of selected chemical reactions found to occur in rockets and jets.

The data sheet format is now firmly established. A total of 34 data sheets have been compiled to date. In addition several manuscripts have been written. Some have been published as internal reports, and the rest have or will appear in outside journals including the Journal of Physical and Chemical Reference Data. Future efforts will be devoted to the production of new data sheets describing the reacting systems: boron-flourine, hydrogen-organics, oxygen-organics, hydrogen-halogens, nitrogen-flourine.

WATER SOLUBILITY AND RELATED PARAMETERS OF COAL DERIVED COMPOUNDS

Sujit Banerjee
Syracuse Research Corporation
Syracuse, New York
Source of Support: DOE and NSF

Data on the water solubility of polynuclear aromatic and heteroaromatic compounds derived from coal will be compiled and evaluated. The evaluated data will be checked against selected theoretical models to establish a relationship between experimental solubility values and those calculated from chemical structure parameters.

The project has been delayed due to the need for more experimental data. When completed, the data will be used for comparison with theoretical model results. These comparisons will be incorporated in the final manuscript.

A CRITICAL COMPILATION OF THE SOLUBILITY OF OXYGEN, OZONE, AND NITROGEN IN LIQUIDS

Rubin Battino
Wright State University
Dayton, Ohio
Source of Support: NSF

This project involves the preparation of data sheets giving the solubility of oxygen, ozone, and nitrogen in liquids, including liquid mixtures, over a range of pressure. These data will be evaluated, and smoothed recommended values will be produced.

To date a manuscript on oxygen and ozone solubilities in water and seawater has been accepted for publication in the Journal of Physical and Chemical Reference Data. Another manuscript on the solubility of nitrogen and air will be completed in the coming year.

SOLUBILITY OF THE SPARINGLY SOLUBLE SALTS OF ZINC, CADMIUM, AND MERCURY IN WATER AND AQUEOUS SALT SYSTEMS

H. Lawrence Clever
Emory University
Atlanta, Georgia
Source of Support, NSF

A compilation containing evaluated data on the solubility of zinc, cadmium, and mercury salts in water and aqueous electrolyte solutions will be prepared. The anions of interest include the halides, sulfides, sulfates, phosphates, and carbonates at all temperatures and pressures. In addition, an annotated bibliography on all the other anions for which data are available will be assembled.

To date, the survey of the literature and the collection of all the papers has been completed. The data on the mercury salts are now being extracted and their evaluation will be carried out soon thereafter. Completion of this phase of the work will be followed by the examination of zinc and cadmium salt data.

COMPILATION OF SPECTROSCOPIC DATA BELOW 2000 ANGSTROMS

Raymond L. Kelly
Spectroscopic Data Center, Naval Postgraduate School
Monterey, California
Source of Support, NSF

The project has been established to permit the completion of a compilation of atomic spectral lines with wavelenghts below 2000 Angstroms. In the past year, tables containing the wavelength, intensity, and classification for all lines observed in solar and terrestrial sources as reported in the literature have been assembled. Data for 26 elements were revised and updated.

The data on K through Zn is to be completed by the end of 1982. There is some discussion regarding an update of the elements H through Ar followed by a merger of all the data into one publication for H through Zn. If this plan is adopted the manuscript will be completed in mid 1983.

K SHELL IONIZATION BY HYDROGEN AND HELIUM IONS

Gregory Lapicki
East Carolina University
Greenville, North Carolina
Source of Support: DOE

A comprehensive compilation of x-ray (K shell) production cross sections of hydrogen and helium ions on the elements helium through uranium will be assembled. For each target element the cross sections will be listed according to projectile energy, claimed uncertainties in the results, and target type (gas, solid, thick or thin, etc.). The experimental cross sections will be compared with theoretically derived values.

To date, the literature has been collected through March 1982. Some preliminary efforts have been initiated in computer programming for manipulation of the data and their comparison with theory.

CRITICAL EVALUATION OF CHEMICAL KINETIC DATA FOR METASTABLE ELECTRONICALLY EXCITED SPECIES

K. Schofield
ChemData Corporation
Santa Barbara, California
Source of Support: DOE

A critical evaluation will be performed on the available chemical kinetic rate data for the gas phase reactions of selected electronically excited species. In all, 19 species will be reviewed. They include excited states for NH, O_2, CN, C_2, CH NO, I, and N_2. The data will be presented in a format similar to a previous publication on the subject and will also indicate where additional data are required.

The available data on all but two of the molecules, NO and N_2, have been evaluated. Because of the large body of literature which exists on these molecules, delivery of the final manuscript will not take place until late in 1983.

A CRITICAL COMPILATION OF PROPERTIES DATA ON NONAQUEOUS SOLVENTS IMPORTANT TO BATTERY DEVELOPMENT

R. P. T. Tomkins
New Jersey Institute of Technology
Newark, New Jersey
Source of Support: DOE

A Critical compilation of data on the transport and thermodynamic properties, kinetics, surface and structural aspects, and performance will be produced. Compounds examined will include those of lithium, calcium, and sodium in electrolytes such as sodium polysulfides, antimony trichloride, sulfur dioxide, thionyl chloride, and selected organic solvents. The data will be recorded both at ambient and high temperature.

Collection of data from the literature has proceeded and data for the systems; Li-SO_2, Li-$SOCl_2$, Li-SO_2Cl_2, Li-TiS_2, and Li-organic solvent are now in hand. These will be evaluated while the data for the other systems are accumulated.

PROPERTIES OF ELECTROLYTE SOLUTIONS

Bert Staples
Aqueous Electrolyte Data Center, NBS
Source of Support: DIPPR

Design-oriented calculation methods are being developed for electrolyte systems, and critically evaluated data are being compiled for specific systems. The purpose is to provide a "data book" of thermodynamic data and recommended procedures for calculation. Three classes of problems are under consideration: vapor-liquid-equilibrium calculations for industrially important systems such as SO_2-H_2O and CO_2-H_2O; prediction of precipitation for heavy metal systems such as hydroxide precipitation of chromium; prediction of gypsum precipitation under varying conditions of concentration, temperature, ionic strength, and pressure.

A procedure has been developed for the calculation of the vapor-liquid equilibrium composition of solutions of weak, volatile compounds such as the system SO_2 + H_2O and the equilibrium vapor phases. The procedure involves an intricate, self-consistent calculation involving equilibria both in the gas phase and in solution.

Recommended values have been prepared for the solubility of gypsum, $CaSO_4.2H_2O$, as a function of temperature and added salt concentration. It has been shown in this work that the theoretical treatment of salt mixtures developed by Pitzer reproduces the experimental data very well and, in this case, is better than other approaches. This work has been done to provide evaluated data and calculational example for a handbook being prepared by the Design Institute for Physical Property Data (AIChE). It is also pertinent for coal/flue gas cleanup systems.

PREPARATION OF POURBAIX DIAGRAMS FOR SELECTED SYSTEMS

Marcel Pourbaix
Belgian Center for Corrosion Study
Brussels, Belgium
Source of Support: DOE

Reports are being prepared on the influence of temperature and pressure on the chemical and electrochemical equilibria of the systems O, H, Fe, O-H, O-Fe, H-Fe, O-H-Fe, C, O-C, C-Fe, O-C-Fe. This project is part of a larger program on chemical equilibria involved in corrosion processes.

At the present time, the system O-H has been completed. A second report on Fe-O-H has been prepared, however, it is hoped that better data will be found for the ferric oxides and hydrated ferric oxides. A preliminary report on the potential-pH equilibrium diagrams for the Fe-H_2O system has also been prepared.

THERMODYNAMICS IN HIGH-TEMPERATURE PROCESSES

D. L. Hildenbrand with L. Brewer, G. M. Rosenblatt, D. Cubicciotti
SRI International
Menlo Park, California
Source of Support: DOE

Reports are being prepared on the vaporization behavior of 50 binary oxide systems including vapor composition and thermodynamic properties of condensed and gaseous oxides. These oxides are important for a wide range of industrial uses including metallurgy, high-temperature applications of construction materials, batteries, nuclear reactors, and glass making.

Preliminary reports on the gaseous oxides have already been received.

PROPERTIES OF POLAR FLUIDS

L. Haar, J. M. H. Levelt Sengers
Center for Chemical Engineering, NBS
Source of Support: NBS

A publication of the new formulation on the thermodynamic properties of water and steam is in press. A complete documentation of the formulation is in preparation.

Papers have been prepared on the thermodynamic behavior of water and steam in the critical region and on the transport properties of water and steam and heavy water and steam in the critical region.

A formulation for H_2S is being developed, and work has started on using the HGK formulation, which has been very successful for water in the development of a treatment for mixtures.

THERMOPHYSICAL PROPERTIES DATA FOR FLUIDS

J. V. Sengers
University of Maryland, College Park, Maryland
Source of Support: NSF

This project is concerned with the development of comprehensive formulations for the thermodynamic and transport properties of fluids. This includes formulations providing an accurate description of the behavior in the critical regions. The techniques are being applied to the properties of water and steam as part of an international effort under the IAPS.

A study on the problems with the Prandtl Number of steam has been completed and published. Work continues on the development of superior formulations for the transport properties of steam in both the classical region and the scaled region near the critical point.

THERMODYNAMIC PROPERTIES OF AIR AND ITS COMPONENTS

R. B. Stewart, R. T. Jacobsen
University of Idaho, Moscow, Idaho
Source of Support: DOE

Extended BWR formulations have been developed for oxygen, nitrogen and argon and are being developed for air. The same equation has been used in each case; the formulations differ only in the values of the coefficients used.

The data available for air and for other compositions of the components of air, such as are found in liquefaction plants, have been collected and evaluated. The extent to which the properties of air can be predicted by using combinations of the single-substance formulations will be examined. The evaluation will specifically include the two-phase region.

THERMODYNAMIC PROPERTIES OF ETHYLENE

R. T. Jacobsen, R. B. Stewart
University of Idaho, Moscow, Idaho
Source of Support: DOE

A comprehensive re-evaluation of the experimental data for ethylene has been carried out in cooperation with the Fluid Mixtures Data Center at NBS Boulder. New improved formulations for the thermodynamic properties of ethylene have been developed. Further work is going on in an attempt to devise a classical formulation that will accurately approach nearer to the non classical region around the critical point than is now possible.

THERMODYNAMIC PROPERTIES OF COAL CHEMICALS

K. R. Hall, R. Wilhoit
Thermodynamic Research Center
Texas A&M University
College Station, Texas
Source of Support: IGT

Data on the thermodynamic properties of fluids are prepared for inclusion in the "Coal Conversion Systems Technical Data Book," a book which the Institute for Gas Technology (IGT) is preparing for DOE.

THERMODYNAMIC PROPERTIES OF KETONES

Buford D. Smith
Thermodynamics Research Laboratory
Washington University
St. Louis, Missouri
Source of Support: NSF

A comprehensive compilation and evaluation has been made on selected thermodynamic properties of ketones. The ketones studied are components in binary systems for which thermodynamic data exist. The properties evaluated are those needed in the evaluation and prediction of mixture data. The work is closely coordinated with the studies of mixture properties being carried out at the same Center.

The compilation and evaluation have been completed. Work on presenting the evaluated data in suitable compact equation form is being carried out.

DIPPR DATA PROJECTS

AIChE
New York, New York
Source of Support: NBS, Industry

DIPPR supports a number of data compilation, evaluation, and prediction projects with cooperative funding from industry and Government. In accordance with an agreement between NBS and AIChE, the parent organization of DIPPR, DIPPR and NBS will cooperate in a variety of ways in the production of critically evaluated data for industry. NBS is providing funds to DIPPR which are being used to support a data prediction manual and a project on electrolyte phase equilibria.

The first five chapters of the data prediction manual have been completed and are in review.

EQUILIBRIUM AND TRANSPORT PROPERTIES OF NOBLE GASES AND THEIR MIXTURES AT LOW DENSITIES

J. Kestin, E. A. Mason
Brown University
Providence, Rhode Island
Source of Support: NSF

This project is designed to exploit recently developed techniques to obtain intermolecular potentials from experimental data to provide definitive data on the thermodynamic and transport properties of noble gases and their mixtures.

The calculations have been completed and a report is being prepared.

DATA ON AQUEOUS ELECTROLYTES

R. Wood
University of Delaware
Newark, Delaware
Source of Support: NSF

This project will be closely coordinated with the work of the Aqueous Electrolyte Data Center. It will focus on the evaluations, coorelation and prediction of data on the thermodynamic properties of aqueous electrolyte solutions. Methods for computerized transfers of various data files between Delaware and NBS will also be investigated.

CATION-NITROGEN DISTANCE IN NITRIDES OF CYRSTALLINE COMPOUNDS

W. H. Baur
University of Illinois - Chicago Circle
Chicago, Illinois
Source of Support: NSF

This project is reviewing and evaluating cation radii for crystalline nitride compounds. It has been found for many crystalline materials that, for a given anion, the cation radius remains the same despite differences in bond types and other structural changes. This has led to useful results, based on an assumption of the additive nature of these radii. However, the cation radii do change for different anions. The cation radii for nitride systems will be reviewed, and an evaluated set of radii will be generated. The nitride compounds have been chosen because of their significance in ceramic materials.

CRYSTALLOGRAPHIC DATA FOR ORGANIC MATERIALS

O. Kennard
Cambridge Crystallographic Data Centre
Cambridge, England
Source of Support: NBS

The Cambridge Crystallographic Data Centre has had a continuing collaboration with the NBS Crystal Data Center. The Cambridge Centre supplies two key sets of information: (1) numerical crystallographic data and references for organic and organomettalic materials, and (2) actual copies of all published crystallographic research on organic materials. The Cambridge Centre has begun to supply the organic entries for the NBS Master Data File in the appropriate format, a major step forward in creating this important file. From these entries, selected information will be used to update the NBS Crystal Data ID File, which is available for on-line use.

During the coming year, emphasis will be placed on completing two new volumes in the series "NBS Crystal Data Determinative Tables" which will contain data on over 20,000 new organic materials.

FUNDAMENTAL PHYSICAL CONSTANTS

E. R. Cohen
Rockwell International - California
Thousand Oaks, California
Source of Support: NSF

Fundamental Physical Constants are those quantities which provide the foundation of our understanding of the physical universe. This project has concerned itself with two important aspects in the analysis of these constants: the "best" values, which are so important for science and technology, in general, and discrepancies among the constants, which are important in defining new measurement needs or improvement in theory or experiment. A part of this effort is the continuing compilation of data for the 1982 adjustment by a CODATA Task Group.

MOLECULAR STRUCTURE AND THERMODYNAMIC PROPERTIES OF ALKALI METAL VAPORS

W. C. Stwalley
University of Iowa
Iowa City, Iowa
Source of Support: NSF

The focus of this project is a compilation of spectroscopic, theoretical, and thermodynamic results on alkali metal molecules and vapors. The first stage is concentrated on spectroscopic constants, dissociative energies, and potential energy curves; the second stage will be a critical review of the thermodynamic properties of the gaseous alkali metal dimers and alkali metal hydride molecules.

OSRD BINARY PHASE DIAGRAM EVALUATION PROJECTS

Rare Earth Alloys

K. A. Gschneidner
Iowa State University
Ames, Iowa
Source of Support: DOE

Copper Alloys

D. E. Laughlin
Carnegie-Mellon University
Pittsburgh, Pennsylvania
Source of Support: NSF

Vanadium and Niobium Alloys

J. F. Smith
Ames Laboratory of DOE
Iowa State University
Ames, Iowa
Source of Support: DOE

Titanium Alloys

J. Murray
National Bureau of Standards
Source of Support: ONR

Alkali Metals

A. Pelton
Thermfact
Montreal, Canada
Source of Support: DOE

These evaluation projects are a major part of the National Bureau of Standards-American Society of Metals (ASM) joint program to provide reliable

phase stability information to the U.S. materials community. The format of all projects is the same. For each binary system a recommended phase diagram will be produced with explanatory text including evaluation of available experimental, crystallographic, and thermodynamic data. The outputs will be published first in the Bulletin of Alloy Phase Diagrams and, as larger numbers of systems are completed, in a series of monographs published by ASM.

The titanium, vanadium, and niobium project are now in their third year, and the rare earth alloys and copper projects are in their second year. A substantial number of binary systems evaluations have been completed.

REFERENCE DATA ON THE REFRACTIVE INDEX OF SELECTED OPTICAL MATERIALS

H. H. Li
CINDAS
Purdue University
West Lafayette, Indiana
Source of Support: DOE

This project has produced recommended reference values for the refractive index of optically important materials, especially those which are serious candidates for use in high-power laser windows and for solar energy applications. The materials to be surveyed include cadmium and zinc sulfides, selenides and tellurides, and certain oxides and halides. All published work on this subject will be reviewed and the data evaluated. A manuscript on the five compounds has been submitted to the Journal of Physical and Chemical Reference Data for publication.

ESCA DATA BASE PROJECT

Charles Wagner
Surfax Compnay
Oakland, California
Source of Support: NSF

Electron Spectroscopy for Chemical Analysis (ESCA) is a technique that has proved of wide importance is characterizing the surface composition of materials. The present project is concerned with creating a data base of critically evaluated line energy data for ESCA. One interesting aspect of this project is the use of a personal computer in building the data base.

Journal of Physical and Chemical Reference Data, Volume 11

A Fundamental Equation of State for Heavy Water
P. G. Hill, R. D. Chris MacMillan, and V. Lee

Volumetric Properties of Aqueous Sodium Chloride Solutions
P. S. Z. Rogers and Kenneth S. Pitzer

Ideal Gas Thermodynamic Properties of CH_3, CD_3, CD_4, C_2D_2, C_2D_4, C_2D_6, C_2H_6, $CH_3N_2CH_3$, and $CD_3N_2CD_3$
K. M. Pamidimukkala, D. Rogers, and G. B. Skinner

Peak Absorption Coefficients of Microwave Absorption Lines of Carbonyl Sulphide
Z. Kisiel and D. J. Millen

Vibrational Contributions to Molecular Dipole Polarizabilities
David M. Bishop and Lap M. Cheung

Energy Levels of Iron, Fe I through Fe XXVI
Charles H. Corliss and Jack Sugar

Microwave Spectrum of Molecules of Astrophysical Interest. XXI. Ethanol (C_2H_5OH) and Propionitrile (C_2H_5CN)
Frank J. Lovas

Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. V. Polystyrene
Umesh Gaur and Bernhard Wunderlich

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry: Supplement I
D. L. Baulch, R. A. Cox, P. J. Crutzen, R. F. Hampson, Jr., J. A. Kerr, J. Troe, and R. T. Watson

Molten Salts Data: Diffusion Coefficients in Single- and Multi-Component Salt Systems
G. J. Janz and N. P. Bansal

JANAF Thermochemical Tables, 1982 Supplement
M. W. Chase, Jr., J. L. Curnutt, J. R. Downey, Jr., R. A. McDonald, A. N. Syverud, and E. A. Valenzuela

Critical Evaluation of Vapor-Liquid Equilibrium, Heat of Mixing, and Volume Change of Mixing Data. General Procedures
Buford D. Smith, Ol Muthu, Ashok Dewan, and Matthew Gierlach

A Compilation of Rate Coefficients for Vibrational Energy Transfer Involving the Hydrogen Halides
Stephen R. Leone

Behavior of the AB_2 Type of Compounds at High Pressure and High Temperatures
Leo Merrill

Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. VI. Acrylic Polymers
Umesh Gaur, Suk-fai Lau, Brent B. Wunderlich, and Bernhard Wunderlich

Molecular Form Factors and Photon Coeherent Scattering Cross Sections of Water
L.R.M. Morin

Chemical Kinetic Data Sheets for High-Temperature Chemical Reactions
N. Cohen and K. R. Westberg

Evaluation of Binary PTxy Vapor-Liquid Equilibrium Data for C_6 Hydrocarbons. Benzene + Cyclohexane
Buford D. Smith, Ol Muthu, Ashok Dewan, and Matthew Gierlach

Evaluation of Binary Excess Enthalpy Data for C_6 Hydrocarbons. Benzene + Cyclohexane
Buford D. Smith, Ol Muthu, Ashok Dewan, and Matthew Gierlach

Evaluation of Binary Excess Volume Data for C_6 Hydrocarbons. Benzene + Cyclohexane
Buford D. Smith, Ol Muthu, Ashok Dewan, and Matthew Gierlach

Thermophysical Properties of Fluids, I: Argon, Ethylene, Parahydrogen, Methane, Nitrogen, Nitrogen Trifluoride, and Oxygen
B. A. Younglove
Supplement I

NBS Tables of Chemical Thermodynamic Properties - Selections for Inorganic and C_1 and C_2 Organic Substances in SI Units
Donald D. Wagman, William H. Evans, Vivian B. Parker, Richard H. Schumm, Iva Halow, Sylvia M. Bailey, Kenneth L. Churney, and Ralph L. Nuttall
Supplement II

NSRDS-NBS Series

Physical Properties Data Compilations Relevant to Energy Storage. V. Mechanical Properties Data on Alloys for Use in Flywheels
Hassell M. Ledbetter
NSRDS-NBS 61 (V)

Rate Constants for Reactions of Aliphatic Carbon-Centered Radicals in Aqueous Solution
Alberta B. Ross and Pedatsur Neta
NSRDS-NBS 70

Ionization Potential and Appearance Potential Measurements, 1971-1981
Rhoda D. Levin and Sharon G. Lias
NSRDS-NBS 71

Tables of Rate Constants for Gas Phase Chemical Reactions of Sulfur Compounds (1971-1980)
Francis Westley
NSRDS-NBS 72

Data Publications from Other Publishers

The Bulletin of Alloy Phase Diagrams, Volumes 2 and 3
Lawrence H. Bennett, Editor
American Society for Metals, quarterly

Diffusion Rate Data and Mass Transport Phenomena in Copper Systems
D. B. Butrymowicz
International Copper Research Association, New York
INCRA Monograph VIII

Equilibrium Properties of Fluid Mixtures: A Bibliography of Experimental Data on Selected Fluids
M. J. Hiza, A. J. Kidnay, and R. C. Miller
IFI/Plenum, New York

Data Publications in Other NBS Series

Heating Values of Natural Gas and Its Components
George T. Armstrong and Thomas L. Jobe, Jr.
NBSIR 82-2401

Interactive FORTRAN Program to Calculate Thermophysical Properties Of Seven Fluids
Benjamine A. Younglove
NBS Technical Note 1048

Medical Physics Data Book
Thomas N. Padikal and Sherman P. Fivozinsky
NBS Handbook 138

Numerical Comparisons of Several Algorithms for Treating Inconsistent Data in a Least-Squares Adjustment of the Fundamental Constants
B. N. Taylor
NBSIR 81-2442

Photonuclear Data Index, 1973-1981 (Supplement 2 to NBS Special Publication 380)
E. G. Fuller and Henry Gerstenberg
NBSIR 82-2543

Other Publications in NBS Series

Technical Activities 1982, Office of Standard Reference Data
Sherman P. Fivozinsky
NBSIR 82-

Bibliographies and Indexes from Other Publishers

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Volume 14, 1981
Radiation Chemistry Data Center
Radiation Laboratory
University of Notre Dame
Notre Dame, IN46556

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Volume 15, 1982

Radiation Chemistry Data Center
Radiation Laboratory
University of Notre Dame
Notre Dame, IN 46556

Bulletin of Chemical Thermodynamics, Volume 25, 1982
IUPAC Commission on Thermodynamics and Thermochemistry
Robert D. Freeman, Editor

Mossbauer Effect Data Index Covering the 1977 Literature
John G. Stevens and Virginia E. Stevens
IFI/Plenum, New York

Machine Readable Data Bases

NBS Chemical Thermodynamics Database
Magnetic data tape available from the Office of Standard Reference Data; available on-line via the NIH/EPA Chemical Information System (CIS)

NBS Crystal Data Identification File
Magnetic tape available from the JCPDS-International Centre for Diffraction Data; available on-line via the NIH/EPA Chemical Information Service (CIS)

NBS/NIH/EPA/MSDC Mass Spectral Database
Magnetic data tape available from the Office of Standard Reference Data; available on-line via the NIH/EPA Chemical Information System (CIS)

Thermophysical Properties of Hydrocarbon Mixtures
Magnetic data tape available from the Office of Standard Reference Data

PUBLICATIONS SCHEDULED FOR 1983

Journal of Physical and Chemical Reference Data, Volume 12

Electrical Resistivity of Ten Selected Binary Alloy Systems
C. Y. Ho, M. W. Ackerman, K. Y. Wu, T. N. Havill, R. H. Bogaard, R. A. Matula, S. G. Oh, and H. M. James

Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. VII. Polyester and Polyamides
Umesh Gaur, Suk-fai Lau, Brent B. Wunderlich, and Bernhard Wunderlich

Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. VIII. Other Carbon Backbone Polymers
Umesh Gaur, Brent B. Wunderlich, and Bernhard Wunderlich

Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. IX. Final Group of (Aromatic and Inorganic) Polymers
Umesh Gaur, Suk-fai Lau, and Bernhard Wunderlich

Carbon Monoxide Thermophysical Properties from 68 to 1000 K at Pressures to 100 MPa
Robert D. Goodwin

Thermochemical Data for Gaseous Monoxides
J. B. Pedley and W. M. Marshall

Thermodynamic Properties of Steam in the Critical Region
J. M. H. Levelt Sengers, G. Kamgar-Parsi, F. W. Balfour, and J. V. Sengers

A Survey of Electron Swarm Data in Electro-Negative Gases
J. W. Gallagher, E. C. Beatty, J. Dutton, and L. C. Pitchford

The Solubility of Oxygen and Ozone in Liquids
Rubin Battino, Timothy R. Rettich, and Toshihiro Tominaga

Recommended Data on the Electron Ionization of Light Atoms and Ions
K. L. Bell, H. B. Gilbody, J. G. Hughes, A. E. Kingston, and F. J. Smith

A Correlation of the Viscosity and Thermal Conductivity Data of Gaseous and Liquid Ehtylene
P. M. Holland, B. E. Eaton, and H. J. M. Hanley

Recommended Values for the Thermal Expansivity of Silicon from 0 K to 1000 K
C. A. Swenson

Atlas of the High Temperature Water Vapor in the 3000 to 4000 cm^{-1} Region
A. S. Pine and M. J. Coulombe

Evaluated Theoretical Cross Section Data for Charge Exchange of Multiply Charged Ions with Atoms. I. Hydrogen Atom-Fully Stripped Ion Systems
R. K. Janey, J. W. Gallagher, and B. H. Bransden

Molten Salts: Volume 5, Part 2
G. J. Janz and R. P. T. Tomkins

Transport Properties of Liquid and Gaseous D_2O in a Wide Range of Temperature and Pressure
N. Matsunaga and A. Nagashima

Thermodynamic Properties of D_2O in the Critical Region
B. Kamgar-Parsi, J. M. H. Levelt Sengers, and J. V. Sengers

Evaluated Theoretical Cross Section for Charge Exchange of Multiply Charged Ions with Atoms. II. Hydrogen Atom Partially Stripped Ion System
J. W. Gallagher, B. H. Bransden, and R. K. Janey

Evaluation of Binary PTxy Vapor-Liquid Equilibrium Data for C_6 Hydrocarbons. Benzene + Hexane.
Buford D. Smith, Ol Muthu, and Ashok Dewan

Evaluation of Binary Excess Enthalpy Data for C_6 Hydrocarbons. Benzene + Hexane.
Buford D. Smith, Ol Muthu, and Ashok Dewan

Evaluation of Binary Excess Volume Data for C_6 Hydrocarbons. Benzene + Hexane.
Buford D. Smith, Ol Muthu, and Ashok Dewan

Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon range C_1 to C_4, Part 1. Properties of Condensed Phases
R. C. Wilhoit, J. Chao, and K. R. Hall
Supplement II

Heat Capacity, Entropies, and Some Phase Transition Properties of Organic Compounds in the Liquid and Solid Phases
E. S. Domalski, W. H. Evans, and E. D. Hearing
Supplement I

NSRDS-NBS Series Scheduled

Selected Tables of Atomic Spectra: A. Atomic Energy Levels Second Edition; B. Multiplet Tables; O III
Charlotte E. Moore
NSRDS-NBS 3 (11)

Selected Tables of Atomic Spectra: A. Atomic Energy Levels - Second Edition; B. Multiplet Tables; O II
Charlotte E. Moore
NSRDS-NBS 3 (12)

Data Publications Scheduled from Other Publishers

A Compilation of Depth-Dose Data from Medical Linear Accelerators
J. A. Purdy, W. B. Harms, and S. P. Fivozinsky
American Association of Physicists in Medicine

Steam Tables: 1982
Lester Haar, John S. Gallagher, and George S. Kell
Hemisphere Press

Other Publications Scheduled for NBS Series

A Thermodynamic Surface for the Critical Region of Ethylene
J. M. H. Levelt Sengers, J. S. Gallagher, F. W. Balfour, and J. V. Sengers
NBS Technical Note

A Program to Simulate a Normal Distribution: The Galton Quincunx
Joseph Hilsenrath and Bruce F. Fields
NBSIR 82-2515

Bibliographies and Indexes Scheduled from Other Publishers

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Volume 15, 1982
Radiation Chemistry Data Center
Radiation Laboratory
University of Notre Dame
Notre Dame, IN 46556

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Volume 16, 1983
Radiation Chemistry Data Center
Radiation Laboratory
University of Notre Dame
Notre Dame, IN 46556

Bulletin of Chemical Thermodynamics, Volume 26, 1983
IUPAC Commission on Thermodynamics and Thermochemistry,
Robert D. Freeman, Editor

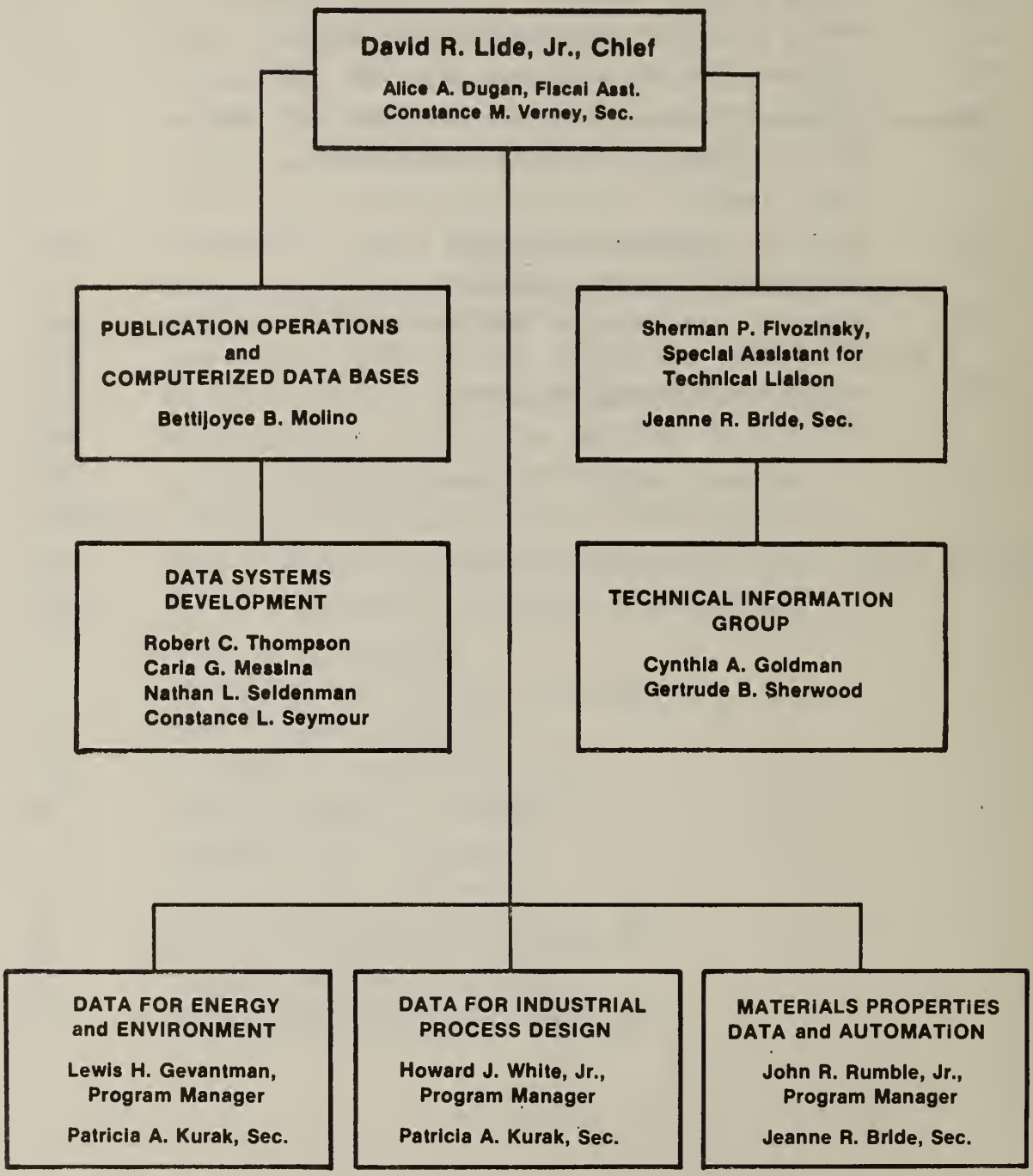
LIST OF ACRONYMS AND ABBREVIATIONS

AAAS	American Association for the Advancement of Science
AAPM	American Association of Physicists in Medicine (AIP)
ACerS	American Ceramic Society
ACS	American Chemical Society
ADP	Automatic data processing
AIChE	American Institute of Chemical Engineers
AIME	American Institute of Mining, Metallurgical, and Petroleum Engineers
AIP	American Institute of Physics
API	American Petroleum Institute
APS	American Physical Society (AIP)
ASM	American Society for Metals
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
BAPD	Bulletin of Alloy Phase Diagrams
BRS	Bibliographic Retrieval Services, Inc.
BWR	Benedict-Webb-Rubin (formulation)
CAC	Center for Analytical Chemistry, NML, NBS
CAPQ	Center for Absolute Physical Quantities, NML, NBS
CCE	Center for Chemical Engineering, NEL, NBS
CCF	Central computing facility
CCP	Center for Chemical Physics, NML, NBS
CINDAS	Center for Information and Numerical Data Analysis and Synthesis, Purdue University
CIS	Chemical Information System (NIH/EPA)
CMS	Center for Materials Science, NML, NBS
CODATA	Committee on Data for Science and Technology (ICSU)
CRR	Center for Radiation Research, NML, NBS
CSIN	Chemical Substances Information Network (EPA)
DARPA	Defense Advanced Research Projects Agency
DEAP	Division of Electron and Atomic Physics (APS)
DIPPR	Design Institute for Physical Property Data (AIChE)
DOE	U.S. Department of Energy
EEO	Equal Employment Opportunity

EPA	U.S. Environmental Protection Agency
ESCA	Electron spectroscopy for chemical analysis
FDA	Food and Drug Administration
FY	Fiscal year
GIIGNL	Groupe International des Importateurs de Gaz Naturel Liquefie
GPE	General purpose equipment
GRI	Gas Research Institute
HGK	Haar-Gallagher-Kell (formulation)
IAPS	International Association for the Properties of Steam
ICRU	International Commission on Radiation Units and Measurements
ICSU	International Council of Scientific Unions
IFC	International Formulating Committee (IAPS)
INCRA	International Copper Research Association
ISTT	Internationalization and Systematization of Thermodynamic Tables (CODATA Task Group)
IUPAC	International Union of Pure and Applied Chemistry (ICSU)
JANAF	Joint Army, Navy, Air Force (historical acronym)
JCAMP	Joint Committee on Atomic and Molecular Physical Data
JCPDS	Joint Committee on Powder Diffraction Standards
JCPDS-ICDD	JCPDS-International Centre for Diffraction Data
JILA	Joint Institute for Laboratory Astrophysics, NML, NBS-U. of Col.
JPCRD	Journal of Physical and Chemical Reference Data
LET	Linear energy transfer
LLL	Lawrence Livermore National Laboratory
MPC	Metal Properties Council
MSDC	Mass Spectral Data Centre (UK)
NAS	National Academy of Sciences
NBS	National Bureau of Sciences
NDE	Non-destructive evaluation
NEL	National Engineering Laboratory, NBS
NIH	National Institutes of Health
NML	National Measurement Laboratory, NBS

NRC	National Research Council
NSF	National Science Foundation
NSRDS	National Standard Reference Data System
OA	Other agency (funding)
ONR	Office of Naval Research
ONWI	Office of Nuclear Waste Isolation, Battelle
OSRD	Office of Standard Reference Data, NML, NBS
OSRM	Office of Standard Reference Materials, NML, NBS
PDFC	Phase Diagrams for Ceramists Data Center
PL	Public law
RCDC	Radiation Chemistry Data Center
RPI	Rensselaer Polytechnic Institute
STRS	Scientific and Technical Research and Services (appropriated NBS funds)
USGS	United States Geological Survey

OFFICE OF STANDARD REFERENCE DATA



STAFF OF THE OFFICE OF STANDARD REFERENCE DATA

Chief - Dr. David R. Lide, Jr.
Secretary, Ms. Constance M. Verney
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Overall management of the program; Editor-in-Chief of NSRDS publications

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PUBLICATIONS BY OSRD STAFF

Medical Physics Data Book, T. N. Padikal and S. P. Fivozinsky, Editors, NBS Handbook 138

The Development and Use of Numeric Physical/Chemical Properties Databases, S. P. Fivozinsky, Drexel Library Quarterly, 18 (1982).

Physical Properties Data for Basalt, L. H. Gevantman, Editor, NBSIR 82-2587

Ionization Potential and Appearance Potential Measurements, 1971-1981, Rhoda D. Levin and Sharon Lias, NSRDS-NBS 71

Chemical Physics, D. R. Lide, Jr., The Encyclopedia of Physics, 3rd Edition, R. M. Besancon, Editor, Van Nostrand Reinhold Co., Dayton, Ohio; in press

Chapter 8: Atomic and Molecular Properties, D. R. Lide, Jr., CODATA Directory of Data Sources for Science and Technology, Pergamon Press (1982)

Activities of the Office of Standard Reference Data in Relation to the Online Distribution of Scientific Numerical Data, Bettijoyce Molino, John Rumble, and David Lide, Proceedings of the Third National Online Meeting, New York (March 1982)

Computerized Standard Reference Data, Bettijoyce B. Molino, Proceedings of the 6th International Conference on Computers in Chemical Research and Education (1982)

State-to State Differential Cross Sections for Vibrational-Rotational Excitation and Elastic Scattering of Electrons by N_2 at 5-50 eV: Calculations Using Extended-Basis-Set Hartree-Fock Wavefunction, J. R. Rumble, Jr. and D. G. Truhlar, J. Chem. Phys. (submitted)

A Systematic Approach to the Preparation of Thermodynamic Tables, Report of the CODATA Task Group on Internationalization and Systematization of Thermodynamic Tables, Howard J. White, Jr., (Chairman), CODATA BULLETIN No. 47, Pergamon Press (May 1982)

INVITED TALKS AND PRESENTATIONS BY OSRD STAFF

Future Use Patterns of Numeric Scientific Data Bases - Can We See What's Coming?, ASIS 45th Annual Meeting, Columbus, OH, October 1982
Sherman P. Fivozinsky

Physical Properties Data of Rock Salt for Use in Designing Nuclear Waste Repositories, Process Minerology Symposium, AIME Meeting, Dallas, TX, February 1982
Lewis H. Gevantman

Recommended Practices Regarding Symbols, Units, and Data Presentation, Conference of American Chemical Society Editors, Tucson, AZ, January 1982
David R. Lide, Jr.

Quality Assurance in Physical Science Data Bases, Workshop on Data Quality Indicators, NBS and Chemical Manufacturers Association, NBS, Washington, DC, February 1982
David R. Lide, Jr.

Assuring Data Quality, 11th Mid-Year Meeting of the American Society for Information Science, Knoxville, TN, June 1982
David R. Lide, Jr.

New Modes of Numerical Data Dissemination, 1982 Summer National Meeting, American Institute of Chemical Engineers, Cleveland, OH, August 1982
David R. Lide, Jr.

The Need for Validation of Numerical Data Bases, Symposium on Numerical Data Sources, 184th National Meeting, Division of Chemical Information, American Chemical Society, Kansas City, MO, September 1982
David R. Lide, Jr.

Computerized Standard Reference Data, 6th International Conference on Computers in Chemical Research and Education, Washington, DC, July 1982
Bettijoyce B. Molino

Status of Online Numeric Data Bases in the National Standard Reference Data System, ASIS 45th Annual Meeting, Columbus, OH, October 1982
Bettijoyce B. Molino

Activities of the Office of Standard Reference Data in Relation to the Online Distribution of Scientific Numerical Data, Third National Online Meeting, New York, NY, March 1982
John R. Rumble, Jr.

"Chemical Models and Electron Scattering," Amherst College, Department of Chemistry, April 26, 1982
John R. Rumble, Jr.

"Status and Trends of Numeric Data Banks," Eighth International CODATA Conference, Jachranka, Poland, October 1982
John R. Rumble, Jr.

The ASM/NBS Program of Binary Phase Diagram Evaluation, with T. Massalski and H. Baker, Eighth International CODATA Conference, Jachranka, Poland, October, 1982
John R. Rumble, Jr.

Recent Developments in the Programs of the Office of Standard Reference Data, DIPPR Liaison Committee Meeting in conjunction with the AIChE Annual Meeting, Los Angeles, CA, November 1982
Howard J. White, Jr.

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

David R. Lide, Jr.

Council of the American Physical Society (APS)

Audit Committee, APS (Chairman)

Committee on Fellowships, Division of Chemical Physics, APS

1983 Irving Langmuir Prize Committee, APS (Chairman)

American Institute of Physics (AIP) Publication Board

Committee on Nomenclature, ACS

Division of Physical Chemistry, ACS (Alternate Councilor)

Chemical Abstracts Advisory Board, ACS

Section Committee, Chemistry, AAAS

Petroleum Research Fund Advisory Board, ACS

Journal of Physical and Chemical Reference Data (Editor)

Committee on Data for Science and Technology of International Council of Scientific Unions (Member of Executive Committee)

CODATA Publication Committee (Chairman)

CODATA Bulletin (Associate Editor)

Program Committee for Eighth International CODATA Conference

Joint Committee on Atomic and Molecular Physical Data (JCAMP)

Interdivisional Committee on Nomenclature and Symbols, IUPAC

Commission on Symbols, Terminology, and Units, IUPAC

Physical Chemistry Division, IUPAC (President-Elect)

Chemical Information System (CIS) Steering Committee (Chairman)

NAS/NRC Committee on Atomic and Molecular Science

Lewis H. Gevantman

IUPAC Commission V.8 on Solubility Data (Co-Secretary)

Source Selection Board, Department of the Army, Medical Bioengineering Research and Development Laboratory

Executive Committee, Joint Committee on Atomic and Molecular Physical Data

Subcommittee on the Chemical Substance Information Network (CSIN)

Basic Nuclear Data Committee of the National Nuclear Data Center (Observer)

Reference Nuclear Data Committee of the National Nuclear Data Center (Observer)

Subcommittee on Batteries of the Advisory Committee on Energy Storage to the Department of Energy

Howard J. White, Jr.

International Association for the Properties of Steam (Executive Secretary)

Task Group on the Internationalization and Systematization of Thermodynamic Tables (CODATA/ICSU) (Chairman)

Subcommittee on Thermodynamic Tables, Commission on Thermodynamics, International Union of Pure and Applied Chemistry (IUPAC) (Secretary)

Engineering Sciences Data Unit, Ltd. (Corresponding Member)

Research Committee on the Properties of Steam, American Society of Mechanical Engineers (Secretary)

Design Institute for Physical Properties Data (AIChE)
- Administrative Committee
- Technical Committee (non-voting)
- Liaison Committee
- Data Compilation Project Advisory Committee
- Electrolyte Data Project Advisory Committee

American Petroleum Institute Subcommittee on Technical Data (Advisor)

John R. Rumble, Jr.

Liaison Member, Committee on Materials Information Use in Computerized Structural Design in Manufacturing, National Materials Advisory Board, NAS/NRC

Organizing Committee, Materials Data Workshop, Fairfield Glade, Tennessee (November 1982)

Management Oversight Committee for Metals Properties Council Feasibility Study for Materials Property Data Book

Management Board, NBS/JCPDS-International Centre for Diffraction Data - Joint Project

Sherman P. Fivozinsky

AAPM Medical Physics Data Group

Task Group on Accessibility and Dissemination of Data (CODATA/ICSU) (Secretary)

ASTM Committee (F4) on Medical and Surgical Materials and Devices

Bettijoyce B. Molino

Computer Users Advisory Committee (NBS)

Program Committee for the ACS Chemical Information Division

Alice A. Dugan

NML Administrative Council

NML-EEO Women's Personnel Panel, NBS

NBS SEMINARS SPONSORED BY OSRD

February 10, 1980

The Commission and Its Programs in Improving the Dissemination of Federal Information, Toni Carbo Bearman, National Commission on Libraries and Information Science, Washington, D.C.

March 3, 1982

Current Developments in the Cambridge Crystallographic Database, David G. Watson, Cambridge University, U.K.

May 26, 1982

SI Units and Related Matters - How to Get Your Manuscripts Right the First Time, David R. Lide, Jr., NBS, Washington, D.C.

September 30, 1982

Reference Data Activities in India - Especially with Respect to Water and Steam, Nanoo Jayarajan, Bharat Heavy Electricals Ltd., Ranipur, India

October 13, 1982

Computer Interpretation of Analytical Data with Examples from GC/FTIR, Thomas Isenhour, University of North Carolina, Chapel Hill, N.C.

Public Law 90-396
90th Congress, H. R. 6279
July 11, 1968

An Act

To provide for the collection, compilation, critical evaluation, publication, and sale of standard reference data.

Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,

Standard Reference Data Act.

DECLARATION OF POLICY

SECTION 1. The Congress hereby finds and declares that reliable standardized scientific and technical reference data are of vital importance to the progress of the Nation's science and technology. It is therefore the policy of the Congress to make critically evaluated reference data readily available to scientists, engineers, and the general public. It is the purpose of this Act to strengthen and enhance this policy.

82 STAT. 339

DEFINITIONS

82 STAT. 340

SEC. 2. For the purposes of this Act—

(a) The term "standard reference data" means quantitative information, related to a measurable physical or chemical property of a substance or system of substances of known composition and structure, which is critically evaluated as to its reliability under section 3 of this Act.

(b) The term "Secretary" means the Secretary of Commerce.

Collection and publication of standard reference data.

SEC. 3. The Secretary is authorized and directed to provide or arrange for the collection, compilation, critical evaluation, publication, and dissemination of standard reference data. In carrying out this program, the Secretary shall, to the maximum extent practicable, utilize the reference data services and facilities of other agencies and instrumentalities of the Federal Government and of State and local governments, persons, firms, institutions, and associations, with their consent and in such a manner as to avoid duplication of those services and facilities. All agencies and instrumentalities of the Federal Government are encouraged to exercise their duties and functions in such manner as will assist in carrying out the purpose of this Act. This section shall be deemed complementary to existing authority, and nothing herein is intended to repeal, supersede, or diminish existing authority or responsibility of any agency or instrumentality of the Federal Government.

Standards, etc. Publication in Federal Register.

SEC. 4. To provide for more effective integration and coordination of standard reference data activities, the Secretary, in consultation with other interested Federal agencies, shall prescribe and publish in the Federal Register such standards, criteria, and procedures for the preparation and publication of standard reference data as may be necessary to carry out the provisions of this Act.

Sale of reference data. Cost recovery.

SEC. 5. Standard reference data conforming to standards established by the Secretary may be made available and sold by the Secretary or by a person or agency designated by him. To the extent practicable and appropriate, the prices established for such data may reflect the cost of collection, compilation, evaluation, publication, and dissemination of the data, including administrative expenses; and the amounts received shall be subject to the Act of March 3, 1901, as amended (15 U.S.C. 271–278e).

31 Stat. 1449; Ante, p. 34.

U. S. copyright and renewal rights.

SEC. 6. (a) Notwithstanding the limitations contained in section 8 of title 17 of the United States Code, the Secretary may secure copyright and renewal thereof on behalf of the United States as author or proprietor in all or any part of any standard reference data which

61 Stat. 655; 76 Stat. 446.

he prepares or makes available under this Act, and may authorize the reproduction and publication thereof by others.

(b) The publication or republication by the Government under this Act, either separately or in a public document, of any material in which copyright is subsisting shall not be taken to cause any abridgment or annulment of the copyright or to authorize any use or appropriation of such material without the consent of the copyright proprietor.

Appropriation.

SEC. 7. There are authorized to be appropriated to carry out this Act, $1.86 million for the fiscal year ending June 30, 1969. Notwithstanding the provisions of any other law, no appropriations for any fiscal year may be made for the purpose of this Act after fiscal year 1969 unless previously authorized by legislation hereafter enacted by the Congress.

Short title.

SEC. 8. This Act may be cited as the "Standard Reference Data Act."

Approved July 11, 1968.

LEGISLATIVE HISTORY:

HOUSE REPORT No. 260 (Comm. on Science and Astronautics).
SENATE REPORT No. 1230 (Comm. on Commerce).
CONGRESSIONAL RECORD:
Vol. 113 (1967): Aug. 14, considered and passed House.
Vol. 114 (1968): June 13, considered and passed Senate, amended.
June 27, House concurred in Senate amendments.

GPO 98-139

NSRDS DATA CENTERS

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Atomic Energy Levels Data Center

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*The Office of Standard Reference Data is not involved at the present time in the administration or funding of these data centers but assists in making their outputs and services known to the scientific community.

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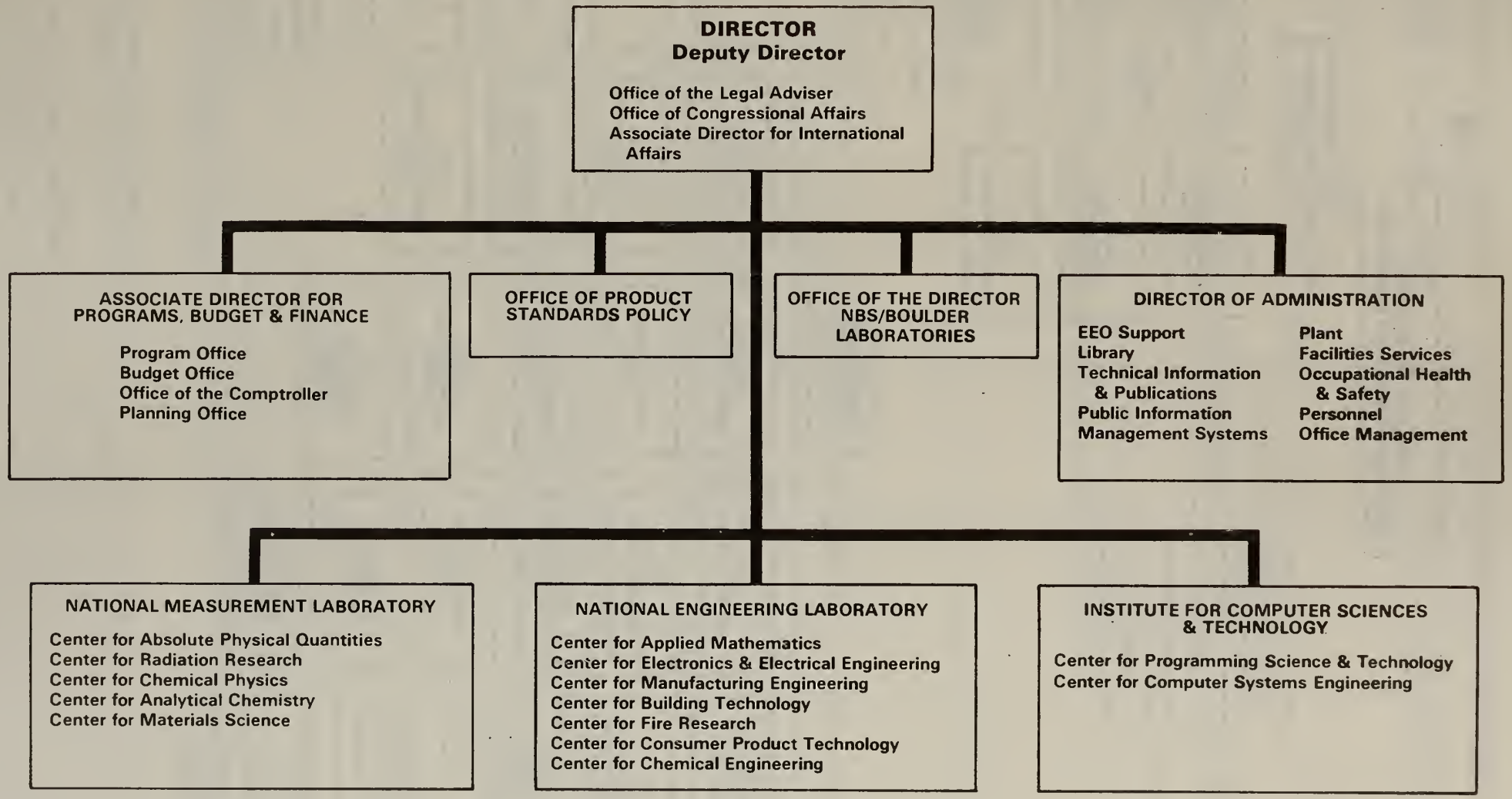

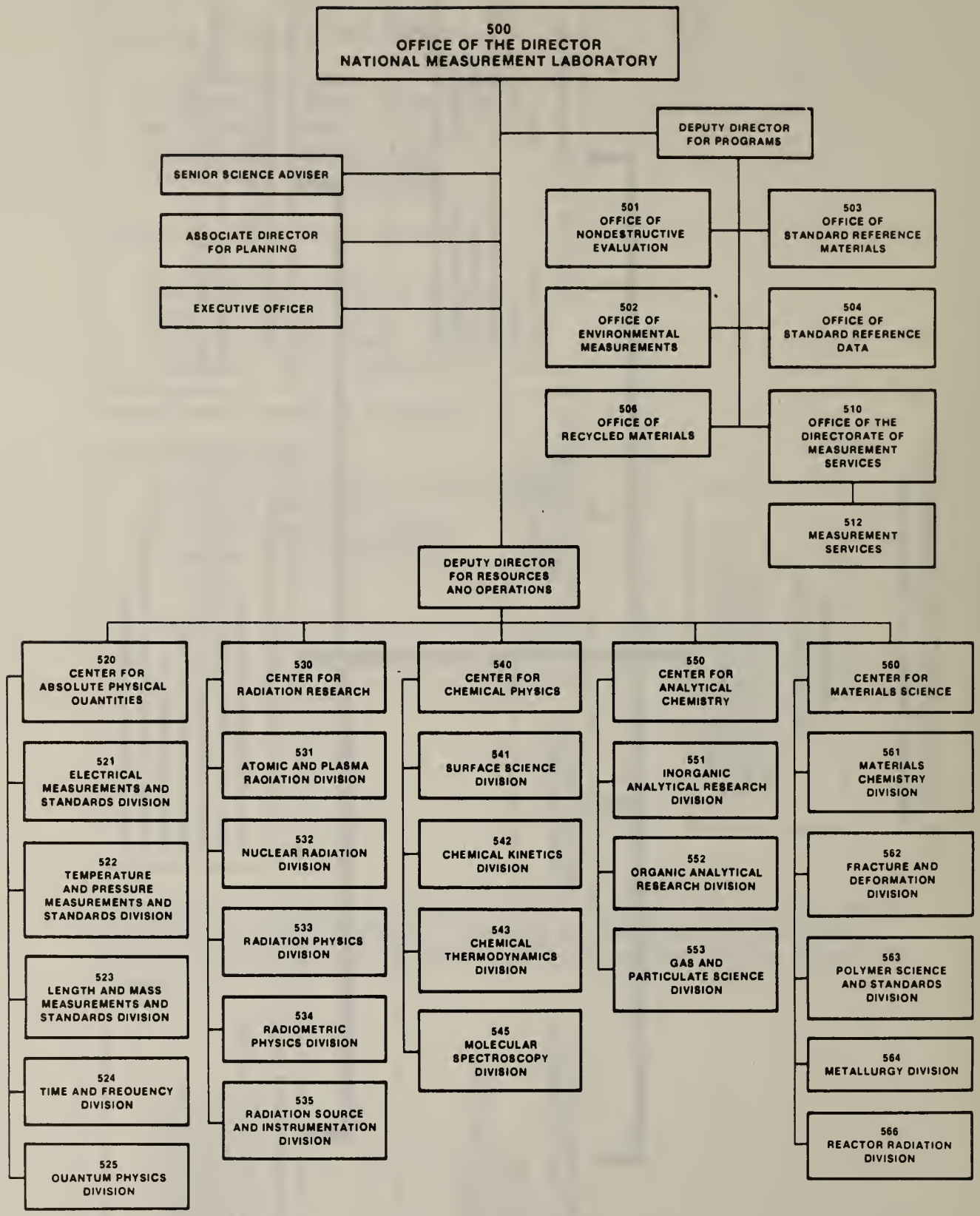
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5. AUTHOR(S)

Sherman Fivozinsky

6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions)

NATIONAL BUREAU OF STANDARDS
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WASHINGTON, D.C. 20234

7. Contract/Grant No.

8. Type of Report & Period Covered

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10. SUPPLEMENTARY NOTES

☐ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

The Office of Standard Reference Data is one of four program offices in the National Measurement Laboratory, National Bureau of Standards. The Standard Reference Data Program develops and disseminates data bases of critically evaluated physical/chemical properties of substances. These data bases are available through NBS and private publications, on magnetic tape, and from on-line retrieval systems.

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1982.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

data compilation; energy and environmental data, evaluated data; materials data; standard reference data; technical activities 1982; thermochemical and thermophysical data.

13. AVAILABILITY

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