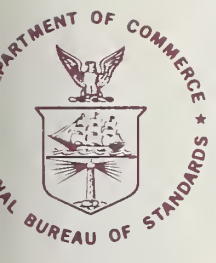

NBS TECHNICAL NOTE 881

U.S. DEPARTMENT OF COMMERCE / National Bureau of Standards

Critical Evaluation of Data in the Physical Sciences —

A Status Report on the National Standard Reference Data System

April 1975

NATIONAL BUREAU OF STANDARDS

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

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

Applied Mathematics — Electricity — Mechanics — Heat — Optical Physics — Nuclear Sciences [2] — Applied Radiation [2] — Quantum Electronics [3] — Electromagnetics [3] — Time and Frequency [3] — Laboratory Astrophysics [3] — Cryogenics [3].

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

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

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[1] Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.
[2] Part of the Center for Radiation Research.
[3] Located at Boulder, Colorado 80302.
[4] Part of the Center for Building Technology.

Critical Evaluation of Data in the Physical Sciences—

A Status Report on the National Standard Reference Data System April 1975

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Washington, D.C. 20234

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Issued September 1975

Library of Congress Catalog Card Number: 75-600066

National Bureau of Standards Technical Note 881

Nat. Bur. Stand. (U.S.), Tech. Note 881, 53 pages (Sept. 1975)

CODEN: NBTNAE

U.S. GOVERNMENT PRINTING OFFICE
WASHINGTON: 1975

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402
(Order by SD Catalog No. C13.46:881). Price $1.10. (Add 25 percent additional for other than U.S. mailing).

PREFACE

The last report on the status of the National Standard Reference Data System appeared more than two years ago. A number of new projects have been started since that time, and major changes have been made in the method of disseminating the output of the program. NSRDS data compilations have played a role in the attack on a number of important national problems. The progress of the system, the plans for the future, and some of the impacts of the programs are summarized in this Status Report.

The National Standard Reference Data System is intended to provide a basic service to the entire scientific and technical community of the United States. The success of the program depends very critically on feedback from the users of the output. We welcome all comments, suggestions, and criticisms on the program.

David R. Lide, Jr.
Chief, Office of Standard Reference Data

STAFF OF THE OFFICE OF STANDARD REFERENCE DATA

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A B S T R A C T

This is a report on the status of the National Standard Reference Data System as of April 1975. Current activities and functions of the Office of Standard Reference Data are summarized. A complete list of data evaluation projects supported by the Office of Standard Reference Data during Fiscal Year 1975 is included; this list also includes projects which received financial support during the previous fiscal year, and which are still actively involved in some aspect of data compilation and evaluation. The list of projects includes continuing data centers in the United States whose activities fall within the scope of the system, but which are not formally affiliated with it. A list of publications resulting from the Standard Reference Data program is provided.

Key words: Atomic and molecular data; chemical kinetics; colloid and surface properties; mechanical properties; nuclear data; standard reference data; solid state data; thermodynamic data, transport properties.

CRITICAL EVALUATION OF DATA IN THE PHYSICAL SCIENCES

A STATUS REPORT ON THE NATIONAL STANDARD REFERENCE DATA SYSTEM

April 1975

I. GENERAL SURVEY

A. Origin of the National Standard Reference Data System

The formal existence of the National Standard Reference Data System 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. The existing data compilation activities supported by NBS and other Government agencies were to be strengthened, new projects started in neglected technical areas, and the entire effort molded into a coherent program.

The technical scope of the program is restricted to well-defined physical and chemical properties of substances and systems which are well-characterized. While this definition leaves some borderline cases, the intent is to concentrate the effort on intrinsic properties which are clearly defined in terms of accepted physical theory. Properties which depend upon arbitrarily defined characteristics of the measurement technique are generally excluded. Likewise, materials of uncertain or variable composition are not included. Biological properties and data relating to large natural systems (e.g., the atmosphere, the oceans) also fall outside the program.

One major aim of the program is to provide critically evaluated numerical data, in a convenient and accessible form, to the scientific and technical community. 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.

B. Organization of NSRDS

When the National Bureau of Standards accepted the primary responsibility for the National Standard Reference Data System, the Office of Standard Reference Data (OSRD) was established at NBS to manage the program. This office is now located under the Associate Director for Information Programs. The OSRD performs several functions. It has the responsibility for allocating that part of the NBS budget which is spent on critical data evaluation, both within the NBS technical divisions and through contracts with outside groups. The staff of the office act as monitors for all projects which are supported. The management of the publications program of NSRDS is also in the hands of OSRD, and an information service is operated on a limited scale. In addition, OSRD maintains close contact with other data compilation activities, both in the United States and abroad. It attempts, both domestically and internationally, to avoid needless duplication and to encourage coverage of all important technical areas. Finally, a small group within OSRD is engaged in research and development on computer handling of data and in application of automated procedures to the activities of data centers.

The actual compilation and evaluation of data takes place in many widely separated groups. It is these groups which form the components of the National Standard Reference Data System. The fact that these groups vary greatly in size, organizational structure, and source of financial support leads to a certain degree of diffuseness in the system. However, it is instructive to recognize two broad types of components in NSRDS. The first is the continuing data center, which has a charter (formal or informal) to cover a certain technical area on a continuing basis. Ideally, such centers have an assurance of stable long-term financial support. The task of a data center is to search the world literature on a regular basis, to retrieve and index papers within its scope of interest, to extract the numerical data, and to carry out critical evaluation leading to publication of tables or reviews. Many of the centers are highly mechanized and have large, computer-based files from which bibliographic citations and data can be retrieved. Generally, they are able to respond to requests for specific information from the scientific public.

The other type of component is the individual scientist (or small group of collaborators) who produces a "one-shot" compilation or critical review as a part of what he regards as his normal scientific activity. Many valuable data compilations have been produced in this way. Such individuals do not consider themselves part of a formal data center, and there is generally no commitment for continuity or updating. The rapid growth of the scientific literature makes it increasingly difficult for an individual to do this type of compilation. However, the continuing data centers can serve a useful function by providing bibliographic back-up for individual scientists in other locations who wish to write critical reviews or do critical compilations of limited scope.

In the pattern which has emerged, it is clear that both types of components are essential for the successful operation of the National Standard Reference Data System. The concentration of the bibliographic phase in a relatively small number of continuing data centers offers many advantages. While these centers carry out some of the critical evaluation of the data, they generally do not have the expertise on their own staff to cover every aspect of the field in question. By enlisting the help of specialists in other institutions for evaluations and critical reviews, the data centers can greatly increase the utilization of their resources.

One of the primary goals of the Office of Standard Reference Data is to establish continuing data centers in all technical areas which fall within the scope of the program. In addition, the office attempts to provide funds for individual compilations and critical reviews of well-defined scope and duration. Since the resources of OSRD are limited, every effort is made to persuade other agencies and private organizations to participate in the support of these activities.

C. Information Resources in OSRD.

1. OSRD Library. The Office of Standard Reference Data has built a broad, although selective, collection of reference data compilations and ancillary publications within the scope of the NSRDS. A list of the holdings was published in September 1970 as NBS Technical Note 554, Annotated Accession List of Data Compilations of the NBS Office of Standard Reference Data. NBS Technical Note 554 listed about 1300 documents. The collection has continued to grow. As of June 30, 1974, the OSRD Library housed over 3000 publications--one of the most extensive holdings of this scope in the world. This is not a lending library, but the use of the documents by visitors within the library is encouraged.

2. Inquiry Services. The Office of Standard Reference Data attempts to answer, within restrictions composed by limited staff and time, inquiries concerning data in the physical sciences and engineering. Information and data are provided from NSRDS publications and other available sources. Inquiries may be referred to data centers and individual specialists in NBS and elsewhere. At times references are provided; if available and appropriate, copies of publications or excerpts therefrom containing the requested data are furnished. OSRD normally receives about 1000 requests and inquiries per year. Under a recently-established cost-recovery program, custom services which require a substantial amount of time are billed to the requestor.

D. Data Systems Design Activities.

The Data Systems Design Group is engaged in computer programming, systems design, and application. Activities of the group focus on the design and application of a number of general-purpose computer programs for storage and retrieval; file manipulation; and computer-assisted text preparation, editing and printing. In the latter area, the Group is working in close collaboration with the Electronic Printing section of the NBS Office of Technical Publications in developing and applying a variety of computer-based systems for more effective use of the Electronic Composing System at the Government Printing Office.

The work includes four main categories:

1. Development of general-purpose computer programs required for the generation and updating of data files and the preparation of publications therefrom.

2. The design of computer-based data files and the associated retrieval systems needed to make them accessible to as wide a segment of the technical community as is economically possible.

3. Consultation and advisory services to the data centers adhering to NSRDS.

4. Source automation of technical manuscripts.

Current activities of the Data System Design Group include:

1. Computer-Assisted Text Editing and File Manipulation.

The writing of general-purpose programs is continuing with the purpose of developing a system of compatible programs which will exploit the capabilities of the newest computer configurations. The programs and the subroutines they require are being written in ANSI Standard FORTRAN IV. The use of a standard FORTRAN and other self-imposed restraints will make it easier to use the programs on a variety of machines.

2. Automatic Typesetting and Composition of Data Tables.

Valuable experience has been gained in writing computer programs to convert existing tapes for automatic typesetting of NSRDS publications. An important consideration in this work is to design the programs insofar as possible for general rather than specific applications. While complete generality has not been achieved, the programs produced thus far have wider applicability than to the documents on which they were used.

3. Applications of the General Purpose Scientific Document Code.

The text handling system based on the General Purpose Scientific Document Code (GPSDC) is now used by most of the NSRDS data centers, including those located away from NBS. Interface programs have been written that permit textual information keyboarded on the ATS text editing system to be converted to GPSDC. This allows the use of a Model 37 teletype with an on-line text-editing system to prepare material to drive the Linotron at the Government Printing Office directly using the GPSDC programs. A program has also been written to convert a GPSDC document to ATS to permit on-line text editing of the material.

4. Source Automation of Technical Manuscripts.

During the calendar year 1973 and 1974 over 20% of the titles published in the Journal of Physical and Chemical Reference Data were prepared for publication using automated procedures which feed more or less directly into computerized typesetting machines. During this same period 50% of the papers of the Office of Standard Reference Data that were published via the Government Printing Office were fully or partially automated.

5. Data Analysis and Retrieval System.

A data analysis and retrieval system named TODARS (Terminal Oriented Data Analysis and Retrieval System) has been written and put into operation. It can be used interactively from an ASCII terminal or in the batch mode. The system is general-purpose in that it can be used on many files. The data fields can be alphabetic and/or numeric. The system is being used to search a number of NSRDS and other NBS data files. TODARS is being used to make the necessary corrections on the Crystal Data tapes, which will be released in the near future. A preliminary version of the users manual has been drafted. After the users have had a chance to comment and the manual has been enlarged and completed, it will be published as an NBS Technical Note.

E. Standard Reference Data Legislation.

The Standard Reference Data Program was established under the general enabling legislation of the National Bureau of Standards. In addition, in 1968 the Congress provided specific legislative authority for the program through passage of Public Law 90-396, the Standard Reference Data Act. The text of the Act is given in Appendix I.

One of the principal features of PL 90-396 is the provision of authority for recovering some of the cost of the program through user charges. In order to make this possible, the Secretary of Commerce is authorized to copyright publications which result from the program and to assign this copyright to others. Several contracts have been negotiated under this authority. In particular, OSRD has contracted with the American Chemical Society and the American Institute of Physics to publish the quarterly Journal of Physical and Chemical Reference Data. This Journal has completed its third year of publication. With the appearance of the last issue of Volume 3, 59 data compilations have been disseminated to users through this medium; in addition, two major compilations have appeared as Supplements. Subscriptions to the Journal and sales of Supplements and individual reprints have provided a useful financial return to the program.

Other channels for cost recovery have also been established. They include:

1. Sale of reports and magnetic tapes through the National Technical Information Service (NTIS).

2. A formal system by which Data Centers charge for custom information and data services.

3. A cooperative undertaking with Plenum Press in the publication of a series of NSRDS-derived bibliographies on specialized topics.

F. Advisory Mechanism.

For good management, the NSRDS program must have reliable feedback from the scientific and technical community. At the time the program was established, the services of the National Academy of Sciences-National Research Council were enlisted for this purpose. The Executive Committee of the Office of Critical Tables of the NAS-NRC provided the focal point for advisory services to the Office of Standard Reference Data. That Office arranged for meetings of advisory panels in the various technical areas, which made recommendations on priorities to OSRD.

As a result of reorganization within the NAS-NAE-NRC, the Office of Critical Tables was replaced in 1969 by the Numerical Data Advisory Board (NDAB). The scope of the NDAB includes numerical data of concern to all parts of science and technology. The NDAB also serves as a focus for coordination with certain other national information programs (such as the National Materials Advisory Board) and international programs parallel to NSRDS. In this latter role, NDAB has responsibility for the US National Committee for CODATA. International undertakings are described more fully in the following section of this report.

The NDAB also administers advisory panels in several of the program areas of NSRDS. These panels meet periodically to discuss needs and priorities within each program area. The membership of the panels is drawn from industry, universities, and Government; an effort is made to achieve coverage of the major specialities within each area. The NDAB submits a report to OSRD after each panel meeting, in which the current activity is appraised and suggestions made for future emphasis.

In addition to the principal advisory panels, ad hoc subpanels are convened at the request of OSRD to discuss problems of a more specific nature. Subpanels of this type have been organized in fields such as Mossbauer spectroscopy, interatomic distances, electrical properties of solids, and thermodynamic properties of aqueous electrolyte solutions. Meetings of such groups have led to the establishment of new compilation projects or (in some cases) to the recommendation of procedures for obtaining and reporting experimental data in the particular field. The NDAB also serves as co-sponsor with OSRD of symposia and conferences on special topics when a broader level of professional interaction appears appropriate to a special subject.

In its broader responsibilities, NDAB is concerned with data outside the physical sciences and with data on less well-defined properties and substances.

G. International Cooperation.

In the period since the establishment of NSRDS, data evaluation activities in other parts of the world have increased considerably. Formal governmental programs similar to NSRDS have been established in several countries. In the U. K., the Science Research Council administers a program which includes the support of a number of data centers in the physical sciences. In the Soviet Union, the Academy of Sciences supports several data evaluation projects, and the State Service for Standard Reference Data (GSSSD) has broad responsibility for scientific and technical data. The Office of Standard Reference Data maintains liaison with these groups with the aim of avoiding duplication in data compilation projects and promoting maximum compatibility of output. Proposals requesting support of projects in subject areas of mutual concern are exchanged for comments.

The establishment of the Committee on Data for Science and Technology (CODATA) in 1966 has provided a formal framework for international cooperation. CODATA is a committee of the International Council of Scientific Unions (ICSU) and contains representation from twelve international unions and, at present, fifteen countries, plus two associated organizations. The Secretariat is located in Paris. The main purpose of CODATA is to encourage, on a world-wide basis, the production and distribution of critically evaluated numerical data. One of its first tasks was to publish an International Compendium of Numerical Data Projects (Springer-Verlag, New York--Heidelberg-Berlin, 1969). This volume lists identifiable data compilation projects throughout the world, with information on their scope, mode of operation, and form of dissemination of output. A revision is in progress.

CODATA has established task groups in a number of special areas, including computer handling of numerical data, publication guidelines for presentation of data, accessibility and dissemination of data, key values of thermodynamic properties, chemical kinetics, and fundamental physical constants. On the basis of immediate scientific impact, two products of CODATA task groups stand out. The first is the adoption and publication of standard values for thermodynamic properties of certain key substances. These internationally-endorsed values will increase the level of consistency and compatibility of thermodynamic calculations throughout the world. The second significant result is the adoption in 1973 of a new set of values for the fundamental constants.

In other areas, CODATA task groups have received endorsement and sponsorship by Unesco on topics of common interest. The resources of CODATA are used by Unesco in constructing UNISIST, a proposed world scientific and technical information system. Members of NSRDS data projects and staff members of OSRD have been active in all of the CODATA task groups.

Cooperation with data groups in the Soviet Union has taken place for a number of years under the auspices of international organizations such as CODATA and IUPAC. This interaction has been particularly strong in the area of thermodynamic data, where representatives from the NSRDS Thermochemical Data Center and the Institute for High Temperatures of the Soviet Academy of Sciences have worked together on the establishment of key values of thermodynamic properties. Following the US-USSR agreement on Cooperation in the Fields of Science and Technology, signed May 24, 1972, these interactions have been brought under the jurisdiction of the Joint Commission which supervises the bilateral exchange program. At the present time, Standard Reference Data is one of the items in the Cooperative Program in Metrology.

In addition to the work on key values of thermodynamic properties, there have been close contacts in the areas of thermophysical properties of fluids and chemical kinetics. The interaction has taken the form of exchange of data, exchange of bibliographies and copies of publications, and consultation on formats for computer storage of data. Discussions have taken place on the future possibility of joint preparation of thermodynamic tables, in which data groups in the two countries would work on individual sections which could be merged into the final tables.

II. RECENT ACCOMPLISHMENTS

In the time since the 1972 Status Report appeared, a number of significant advances have occurred in the National Standard Reference Data System. They involve major new data evaluation projects, new cooperative undertakings, added service capabilities, or especially noteworthy data publications. These advances are described briefly below.

Cooperative Project on Ethylene Data

Seven industrial organizations have joined with government and academic laboratories under the program management of the Office of Standard Reference Data to develop a definitive set of thermophysical and related thermodynamic properties of ethylene.

Ethylene is a major item of commerce and is currently produced in the United States at the rate of over 23 billion pounds per year, which ranks it fifth in chemical production. It is used, handled, and transported in the gaseous or liquid state. Such properties as the density of the gas or liquid as a function of temperature and pressure, the extent of the gaseous and liquid regions, the enthalpy, and the heat capacity are needed for handling ethylene in the plant, for equipment design, and for custody transfer. Although there are formulations for these properties which cover limited ranges of pressure and temperature satisfactorily, there is no adequate comprehensive self-consistent set of properties. The new project is designed to fill this need. The project will require experimental measurements and data evaluation. Experimental measurements will be carried out at NBS-Washington, NBS-Boulder Laboratories, the Energy Research Center at Bartlesville, Oklahoma, and the University of Michigan. Data evaluation will be carried out at NBS-Boulder Laboratories.

Financial support will be provided by the Office of Standard Reference Data and the following companies: Celanese Chemical Company, Cities Service Oil Company, Continental Oil Company, Gulf Research and Development Company, Mobil Chemical Company, Monsanto Polymers and Petrochemicals Company and Union Carbide Corporation. It is expected that the project will take five years to complete.

Conference on Data for Energy Research and Development

A conference on Thermodynamics and National Energy Problems was held at Airlie House in Warrenton, Virginia, on June 10-12, 1974. This conference was sponsored by the Office of Standard Reference Data and four other government agencies and held under the auspices of the Numerical Data Advisory Board of the National Academy of Sciences. The purpose of the meeting was to assess the relevance of thermodynamics to the national energy problem and to identify thermodynamic data needed for further development of energy technology.

Survey talks on the current state of the art and identified data needs in various areas were given by recognized experts in this field to set the stage for a series of panel sessions which brought thermodynamicists, technologists, and users together for extended discussions of data needs. The proceedings of the conference have been published by the National Academy of Sciences. These proceedings will be helpful in assessing priorities for funding of future projects.

International Organization for Thermodynamic Tables

A Subcommission on Thermodynamic Tables has been established within the Commission on Thermodynamics of the Physical Chemistry Division of the International Union of Pure and Applied Chemistry. The purpose of the Subcommission is to foster and coordinate data compilation and evaluation activities on subjects in the field of thermodynamics. An immediate concern is the Thermodynamic Tables Project, an activity devoted to the development of tables of thermodynamic properties of industrially important fluids. This project has been active for a number of years and has cooperating projects in several countries. Tables on argon and ethylene have been published and others are nearing publication. Several projects of the Office of Standard Reference Data cooperate with the Thermodynamic Tables Project and a staff member of the OSRD is currently Secretary of the Subcommission.

International Association for the Properties of Steam

Because of the great importance of steam as a working fluid in power generation, the need for internationally accepted values of its properties of high accuracy has been recognized for a long time. Steps to generate internationally accepted tables were initiated 50 years ago and the task is currently the responsibility of the International Conferences on the Properties of Steam and the administrative organization which runs the Conferences and carries out their wishes, the International Association for the Properties of Steam. Several projects of the Office of Standard Reference Data make contributions to the work of the IAPS and a staff member is its Executive Secretary.

Data for Waste Incineration, Part 2

Previous collaboration between the Office of Standard Reference Data and the ASME Research Committee on Industrial and Municipal Wastes resulted in a book, Combustion Fundamentals for Waste Incineration, published in 1974 by ASME under the sponsorship of the Committee. This book, intended to be a handbook for incinerator design and operation, contains a set of thermodynamic tables with detailed instructions on the use of the tables and other thermodynamic calculations in designing and controlling combustion processes for incineration. The tables were prepared by the Chemical Thermodynamic Data Center in the Physical Chemistry Division of the National Bureau of Standards.

A new collaboration has recently been initiated. The tables referred to above cover single substances of well-defined composition. However, materials of complex composition such as newspapers, automobile tires, etc., find their way into incinerators as well. Data on the combustion properties of these materials that are available in the literature will be compiled and evaluated by the Chemical Thermodynamic Data Center and put into tabular form to augment the existing tables and expand their usefulness in incinerator calculations.

Thermal Conductivity of the Elements

A milestone was reached when the Thermophysical Properties Research Center at Purdue completed an evaluation of the thermal conductivities of the elements. This comprehensive study covers all of the elements over the entire temperature range for which data are available. It is published as Supplement No. 1 to Volume 3 (1974) of the Journal of Physical and Chemical Reference Data and titled "Thermal Conductivity of the Elements: A Comprehensive Review." An abridged, somewhat earlier version has also been published (Journal of Physical and Chemical Reference Data, 1, 279, 1972).

Another result was a paper, "Thermal Conductivity of the Elements," published in Science, 14 September, 1973, Volume 181, pages 999-1008. In this paper the authors discussed what they had found out about this field as a result of systematically reviewing the data in it. Several interesting results were obtained. In the decade between this review and the previous systematic compilation of the same data, the recommended values had changed 20% or more for 22 elements. No experimental data were found for 23 elements; most were very rare but calcium and strontum were included. Finally, it was possible to condense the needs for further measurements on a detailed element-by-element basis to two printed pages.

1973 Values for Fundamental Constants

Dr. E. Richard Cohen of Rockwell International and Dr. Barry N. Taylor of the National Bureau of Standards' Institute for Basic Standards have recently redetermined the "best values" of the fundamental physical constants on the basis of a least-squares adjustment of accumulated experimental data. The work was done under the immediate auspices of the Task Group on Fundamental Constants of the Committee on Data for Science and Technology (CODATA), International Council of Scientific Unions. The Task Group served in an advisory capacity. Financial support for the project was shared among Rockwell International, the NBS Institute for Basic Standards and the NBS Office of Standard Reference Data. The new recommended values of the constants and their estimated uncertainties have been officially adopted by CODATA as a consistent set of fundamental constants.

The 1973 adjustment of the fundamental constants is the outcome of a review and analysis of all the experimental and theoretical data that bear on determination of their numerical values. Experimental results and methods were carefully scrutinized and compared. In some cases, later improvements in theory or the detection of overlooked experimental bias revealed the presence of non-negligible errors; and appropriate corrections were worked out, often with the assistance of the original investigators. In the case of the speed of light, all older determinations were discarded in favor of the recent measurements using lasers, whose uncertainty is smaller by a factor of about 75. The analysis also took into account the uncertainties in the standards of measurement as maintained by various national laboratories. An optimum solution is obtained by the least-squares method.

In recommending official adoption of Cohen and Taylor's 1973 adjustment of the constants, the CODATA Task Group noted that:

"The accuracy and consistency of this adjustment are significantly improved with respect to either the 1963 analysis or the 1969 analysis, yet there are critical areas where additional measurements and theoretical calculations are indicated. The most important of these are the proton gyromagnetic ratio (both high and low field measurements) and the fine structure in hydrogen. . ."

Identification of areas where further measurements and theory development are particularly needed is one of the important by-products of the analysis underlying the revision of the constants. Summing up, the Task Group states:

"For the great bulk of physical and chemical data, where consistency of usage and traceability are perhaps as important as accuracy (and with the recognition that absolute accuracy is a prize that will always elude our grasp), these values should serve as a standard reference set for the next several years."

Data for Radioastronomy

The discovery of formaldehyde in the interstellar medium in 1969 created a sudden demand for microwave spectral data. The radioastronomers who needed the data were unfamiliar with microwave spectroscopy and unable to judge the quality of the existing laboratory data. NBS Monograph 70, "Microwave Spectral Tables" (the last volume of which was published shortly before the discovery) immediately became the "bible" of this field. It was the basis for planning virtually all of the searches for other molecules in space and for identifying new spectral lines that were detected.

As the most abundant molecules were detected and cataloged, the need for more extensive and accurate lists of microwave spectral lines became apparent. When one molecule was known to be prevalent in interstellar space (e.g., formaldehyde, methanol), the possibility that a new line detected in a different spectral region belonged to that molecule had to be considered. The lack of reliable laboratory data over a wide spectral range inhibited both the planning of observations and the interpretation of new results. To meet this need, the NSRDS Microwave Data Center has compiled complete spectral charts of the important molecules already observed or believed to be present. Through a critical evaluation of existing laboratory data and the use of theoretical models to extrapolate into spectral regions where no experimental measurements are available, the Center has produced definitive spectral tables with rigorous uncertainty limits. These tables have become basic reference sources in all observatories engaged in studies of interstellar molecules.

The accuracy of the reference data tables is unusually sensitive in these applications. There is a heavy demand for telescope time, and observations must be scheduled far in advance. The time required to search for a given spectral line is directly proportional to the uncertainty in the predicted frequency of that line. The ability to specify this uncertainty with confidence leads to much more efficient use of telescope time.

Although there are only a small number of radioastronomers in the United States, the cost of conducting this research is very high. The construction cost of a typical telescope is about $4 million, and operating costs average $200 per hour. Thus the greater efficiency resulting from the availability of accurate reference data has considerable leverage in increasing the output per research dollar.

Cooperative Efforts to Improve Spectroscopic Data

Continuing focus on upgrading the quality of spectroscopic data (especially in relation to applied and analytical uses) is the concern of the Joint Committee for Atomic and Molecular Properties (JCAMP).

This volunteer organization brings together the users and the generators of atomic and molecular physical data. It cooperates closely with the Office of Standard Reference Data of the National Bureau of Standards in attempting to identify and help fill needs for data that are relevant to national problems. The committee is composed of representatives from the American Chemical Society, American Society for Mass Spectrometry, American Petroleum Institute, American Physical Society, American Society for Testing and Materials, Coblentz Society, Manufacturing Chemists Association, Optical Society of America, Society for Applied Spectroscopy, and the Spectroscopy Society of Canada.

Past activities of the Joint Commission have been directed toward evaluation and publication of evaluated infrared spectra in cooperation with the Coblentz Society, which has now published 5000 evaluated infrared reference spectra. Guidelines for the evaluation, developed by Coblentz Society Board of Managers and published in 1966, have served as a model for subsequent development, now underway by Joint Committee subcommittees, of similar specifications relating to mass spectra and Raman spectra. These documents should be completed and available during 1975. The ultimate aim is that such guidelines will be adopted by all those who generate and publish spectral data, including journal editors, so that the quality of published data will be upgraded and will be assessable by the user.

Kinetics Data for Atmospheric Chemistry

The Chemical Kinetics Information Center (CKIC) has continued to play a key role in attacking problems relating to both the upper and the lower atmosphere. As part of the Climatic Impact Assessment Program (CIAP) set up by the Department of Transportation, CKIC assembled a "standard" set of rate constants for use by modellers investigating the impact of supersonic transport flights on ozone in the stratosphere. Similar input is being provided to studies of the effect of freons on possible ozone depletion. The Center has also actively supported modellers concerned with the urban troposphere, supplying 127 rate constants needed for a model of the real atmosphere in Northern New Jersey.

In a related area, the CODATA Chemical Kinetics Task Group has been promoting a number of efforts concerned with chemical kinetic data. These efforts have culminated in a series of actions, one of which is aimed at upgrading the reporting of kinetic data in the world literature. A report entitled "CODATA Guidelines on Reporting Data for Chemical Kinetics" has been published in CODATA Bulletin No. 13. In addition, the Task Group has been instrumental in convening a symposium entitled "Symposium on Chemical Kinetics Data for the Lower and Upper Atmosphere." The meeting, which was sponsored jointly by CODATA, NBS, Environmental Protection Agency, Department of Transportation, and Stanford Research Institute attacked the kinetic data problems currently encountered in dealing with the natural and polluted atmosphere and the measurements needed to solve those problems which remain.

Solid State Data Center Interactions

The Electronic Properties Information Center (EPIC) was recently transferred to Purdue University to become a unit in the data center complex there, which now consists of the Thermophysical Properties Research Center, the Underground Excavation and Rock Properties Information Center, the Thermophysical and Electronic Properties Information Analysis Center, and EPIC. A consideration of activities to be pursued within the scope of the Centers' program in optical, magnetic and electronic prop-

erties resulted in an examination of cooperative efforts between EPIC and ongoing OSRD sponsored groups. Useful visits were exchanged between representatives from Research Materials Information Center (RMIC) at Oak Ridge, NBS and EPIC to discuss data projects on optical properties of materials. These visits culminated in the formation of a cooperative project for evaluating refractive index data of laser windows and other laser-related materials.

Similarly, representatives of EPIC and the Alloy Data Center met to examine areas of mutual interest in the alloy data field. Although it was clearly established that the two groups' activities did not overlap it was agreed that close liaison be established for the exchange of information which could be of mutual benefit of each Center.

Critical Survey of Mechanical Properties Data Sources

A new series of critically annotated listings of sources of numerical data, including publications and data centers, has been initiated with the publication of NBS Special Publication 396-1, "Critical Surveys of Data Sources: 1. Mechanical Properties of Metals," by R. B. Gavery, R. L. Moore, and J. H. Westbrook, September, 1974, $1.25, SD Catalog No. C13.10:396-1. This series is designed to assist both engineers and scientists in locating the source of numerical data which best meets their particular needs among the many handbooks, data compilations by societies and trade associations, information centers, and other sources. Other surveys in this series now in the process of final review cover electrical and magnetic properties of metals, and properties of ceramics. A survey covering corrosion data has just been initiated, and the feasibility of a survey covering plastics is under study. The emphasis in all cases is on sources of data covering structural and other commercial materials, and the properties used by designers and others using such materials.

Automation of Technical Compendia at the Source

Publications of several NSRDS data centers are now being routinely prepared at the source in machine readable form with dramatic reduction in the costs of typesetting. The Radiation Chemistry Data Center at Notre Dame University has supplied the text and tables of six NSRDS reports on magnetic tape. Four of these reports have been published and two are in process. The Fundamental Vibration Frequencies of Molecules project at the University of Tokyo, Japan, has supplied the tables for three papers in the Journal of Physical and Chemical Reference Data on punched cards using a coding scheme developed by NBS for input to GPSDC. The original cards are saved and updated. They will be used for a consolidated volume to be published in 1975. The material from both centers was processed by programs developed by OSRD to produce a magnetic tape to drive a Linotron phototypesetting machine. The tables for five other papers in the Journal of Physical and Chemical Reference Data were also supplied on magnetic tape and processed by the NBS Computer Assisted Printing Section.

NSRDS Data Files Available for Distribution on Magnetic Tape

The Office of Standard Reference Data has two magnetic tapes available that are for sale by the National Technical Information Service for $250 each. These are:

NBS Magnetic Tape 2, FORTRAN Programs for Text Edition, File Manipulating and Automatic Typesetting, contains blocked card images for a series of FORTRAN programs consonant with NBS Technical Notes #444, #470, #500, and #700 which document FORTRAN programs for data-manipulation and typesetting of technical manuscripts. The Technical Notes are supplied to purchasers of NBS Magnetic Tape 2.

NBS Magnetic Tape 3, Bibliography and Index to the Literature in the NBS Alloy Data Center, is a copy of the NBS Alloy Data Center's annotated bibliographic file as of January 9, 1973 in blocked card images. The following information is provided for each reference: the first author and the Journal citation; main experimental technique; physical properties, materials studied (metals, and alloys, up to quarternary); material composition and temperature at which the work was performed. The format of the card image and the codes used are described in NBS Tech Note 464 which is supplied with the tape.

III. ACTIVE DATA EVALUATION PROJECTS

The scope of the Standard Reference Data program has been divided into seven technical areas for operational convenience: (1) Thermodynamic and Transport Properties, (2) Atomic and Molecular Data, (3) Chemical Kinetics, (4) Solid State Data, (5) Nuclear Data, (6) Colloid and Surface Properties, and (7) Mechanical Properties. This chapter is devoted to progress reports and project listings for these technical areas.

The lists which follow identify both individual, short-term projects and continuing data centers which receive at least a part of their support from the Office of Standard Reference Data. A supplementary list of continuing data centers in the United States which are recognized as part of NSRDS (even though they do not receive direct financial support from NBS) follows the project descriptions in each technical area.

A. THERMODYNAMIC AND TRANSPORT PROPERTIES

The program on thermodynamic and transport properties is primarily structured to provide broadly based sets of data which have utility in many areas of science and technology. However, an important fraction of the program is devoted to specific current data needs. Emphasis has been placed on chemical thermodynamics and in particular the properties of fluids. Efforts are underway to increase coverage of the thermodynamics of solids.

1. Title: Chemical Thermodynamic Data Center

Location: Physical Chemistry Division, NBS, Washington, D.C.
Project Leader: D. Wagman

Description: This center compiles data on the chemical thermodynamic properties of chemical substances on a continuing basis. Data on inorganic and selected organic substances are being evaluated to provide tables of enthalpies, entropies and Gibbs energies of formation in their standard states at 298K. These tables are published periodically in the NBS Technical Note 270 Series.

The center's activities are highly automated. The center provides the inorganic section the overall substance-property index and the final copy for the Bulletin of Thermodynamics and Thermochemistry each year. New techniques for using computer solutions for large sets of equations are being developed to provide self-consistent sets of chemical thermodynamic data. These developments are being carried out jointly with workers in the United Kingdom.

In another cooperative program under the auspices of CODATA, key values for selected substances are being prepared jointly with a group at the Institute for High Temperatures in Moscow under the direction of an international advisory committee.

Current work involves compounds of the actinides and the alkali metals. For the former the center is coordinating its efforts with those of a group working under the sponsorship of the IAEA.

2. Title: Thermodynamic Data for Industrial and Municipal Incinerator Processes

Location: Physical Chemistry Division, NBS, Washington, D. C.
Project Leader: E. Domalski

Description: Tables developed in a previous project were incorporated in a book entitled Combustion Fundamentals for Waste Incineration, sponsored by the ASME Research Committee on Industrial and Municipal Wastes. This book provided thermodynamic information for incinerator designers and process engineers. In particular enthalpy of formation data were provided on materials identifiable by a single stoichiometric formula. However, there are other substances such as wood, newspapers, tires, etc., for which heat of combustion data may be available, and which often are processed through incinerators. This project is designed to extend the tables in the handbook to include data on such materials. The files of the Chemical Thermodynamics Data Center will be used for this project.

3. Title: Thermodynamic Data on Organic Compounds

Location: Texas A & M University, College Station, Texas
Project Leader: B. J. Zwolinski

Description: This is a continuing project to provide reliable and complete data on important organic compounds ,to meet the needs of science in general, and the chemical and petrochemical industries in particular. The present emphasis is on the chloro- and fluoro-derivatives of methane and ethane in the ideal gas state and on a key set of organic oxygen compounds containing one to four carbon atoms per molecule in the solid, liquid and gaseous states. These compounds are key compounds that will serve as a basis for extrapolation and estimation of data for higher molecular weight chemical substances. This Center also prepares the organic sections of the substance-property index and the bibliography of the Bulletin of Thermodynamics and Thermochemistry.

4. Title: Thermodynamic Properties of Polar Fluids

Location: Heat Division, NBS, Washington, D. C.
Project Leader: M. Klein
Address Inquiries to: L. Haar

Description: This project is concerned with the description of the PVT surfaces and derived thermodynamic properties of one component polar fluids. A formulation of the properties of ammonia from the melting line to 750K and to pressures of 10,000 atmospheres has been completed and is being prepared for publication. Work is underway on the ideal-gas properties of water and the data for the gaseous and liquid phases are being examined to determine whether a new formulation for water is needed at this time.

5. Title: Cryogenic Data Center

Location: Cryogenics Division, NBS, Boulder, Colorado
Project Leader: N. A. Olien

Description: The Cryogenic Data Center maintains a thorough and systematic review of the current published report and patent literature of importance in the cryogenic field. Relevant papers are entered into an automated information system which permits speedy and flexible retrospective searching. The Center provides a weekly cryogenic current awareness service and quarterly reports covering liquified natural gas and superconductivity. Users subscribing to the Center's current awareness services or requiring major literature searches numbered more than 1200 in FY '74.

6. Title: PVT and Related Thermodynamic Properties of Ethylene

Location: See below
Project Leader: H. J. White, Jr., Office of Standard Reference Data, NBS, Washington, D. C.

Description: This project is supported jointly by industrial organizations and the government. The goal is a comprehensive, high-quality, self-consistent set of densities and related thermodynamic properties of ethylene. Since the data in the literature do not allow the preparation of such a set to the level of accuracy desired, the project involves selected measurements as well. Various portions of the work will be carried out at NBS laboratories, the ERDA Energy Research Center in Bartlesville, Oklahoma and the University of Michigan. Measurements involved include measurements near the critical point, properties of the compressed liquid, the speed of sound and the heat capacity. Support for the project comes from several industrial corporations, as identified in Section II, Recent Accomplishment; (above).

7. Title: Thermodynamic Properties of Fluids in the Critical Region

Location: Heat Division, NBS, Washington, D. C.
Project Leader: M. Klein
Address Inquiries to: J. M. H. Levelt Sengers

Description: Experimental measurements near the critical point are difficult; properties change abruptly and have unexpected values. Recent theoretical developments have provided superior methods for formulating properties in the critical region. This project has been concerned with the further development of these methods for evaluation of thermodynamic data in the critical region. Techniques have been developed to compare different sets of measurements of the same property and to compare measurements on different thermodynamic properties so that self-consistent formulations in the critical region can be developed.

The data available for ^3He, ^4He, O_2, Xe, CO_2, and H_2O have been evaluated and suitable formulations obtained. Estimated formulations have also been obtained for Ar, Kr, N_2, H_2, CH_4, C_2H_4, SF_6, and NH_3, and compared to available data.

8. Title: Cryogenic Fluid Mixture Properties

Location: Cryogenics Division, NBS, Boulder, Colorado
Project Leader: D. E. Diller
Address Inquires to: M. J. Hiza

Description: This project is devoted to the compilation and evaluation of data on fluid mixtures with emphasis on mixtures of cryogenic fluids. A comprehensive bibliography of data for low temperature phase equilibria, densities and calorimetric measurements has been completed and is in press. Work is currently in progress on compilation, evaluation and correlation of data for selected close-boiling mixtures containing methane, nitrogen and argon. Compilation and evaluation of data on additional systems is underway and the utility of various evaluative and correlating techniques is being studied.

9. Title: Fused Salt Electrochemistry

Location: Rensselaer Polytechnic Institute, Troy, New York
Project Leader: George J. Janz

Description: This center compiles and evaluates data on molten-salt systems. The properties covered are density, electrical conductivity, viscosity, surface tension, reversible electrode potentials and to some extent vapor pressures. At the present time, the first four properties are being covered for binary-salt systems. Reports on halide mixtures are in press and in preparation.

10. Title: Aqueous Electrolyte Data Center

Location: Physical Chemistry Division, NBS. Washington, D. C.
Project Leader: B. R. Staples

Description: The thermodynamic properties of aqueous electrolytes are collected from the literature, organized and used to supply information services, reviewed and evaluated. At present the osmotic and activity coefficients of polyvalent electrolytes are being evaluated. A report on calcium chloride is in preparation and plans call for comprehensive evaluation of the data on 2:1 and 1:2 electrolytes. Work has also begun on compiling data on the dielectric constant of water.

The center cooperates closely with the Chemical Thermodynamic Data Center.

11. Title: High Pressure Data Center

Location: Brigham Young University, Provo, Utah
Project Leader: H. Tracy Hall
Address Inquiries to: Leo Merrill

Description: This Center is concerned with the compilation and evaluation of data on properties of substances at high pressures. Evaluated data have been published on the phase changes and state changes that can be used to define a scale for pressure and on the behavior of the elements at high pressures. The Center also publishes a current awareness service.

Current effort is directed to the evaluation of data on the behavior of compounds at high pressures. Work on AB compounds is nearing completion.

12. Title: Fluid Transport Properties

Location: Cryogenics Division, NBS, Boulder, Colorado
Project Leader: H. J. M. Hanley

Description: This project is concerned with the transport properties of fluids. Recent theoretical developments relating the transport and equilibrium properties of fluids have been used to evaluate experimental data on transport properties and to provide methods for interpolating between and extrapolating limited data sets. These techniques allow development of formulations providing internally consistent sets of data on thermodynamics and transport properties from limited experimental results.

These techniques have already been applied to the monotomic and simple diatomic fluids and are currently being applied to CO_2 and to larger polyatomic molecules. Preliminary investigations of proper methods for evaluating data on the transport properties of binary mixtures of simple fluids have been started.

13. Title: Correlation of Thermophysical Property Data of Fluids

Location: University of Maryland, College Park, Maryland
Project Leader: J. V. Sengers

Description: This project is concerned with the evaluation and correlation of data on the thermodynamic and transport properties of fluids in the neighborhood of the critical point and with the development of needed data-correlating techniques applicable in the critical region. These properties exhibit unique, and, in some cases, large changes as the critical point is approached and require special correlating techniques to reproduce the observed behavior and to develop consistent formulations covering more than one property. It is also necessary that any special techniques used in the critical region merge satisfactorily with classical formulations known to apply well away from the critical point.

14. Title: Thermal Conductivity

Location: Thermophysical Properties Research Center, Purdue University, Lafayette, Indiana
Project Leader: Y. S. Touloukian

Description: This Center compiles data on 8 thermodynamic and transport properties of materials, over the temperature range for which data are available, on a continuing basis. Another center in the same location compiles data on electrical and electronic properties. At the present time data on thermal and electrical conductivity as functions of temperature and composition are being evaluated for selected binary alloys. Data on C_p, viscosity, and thermal conductivity of 73 fluids are also being evaluated.

The following data centers, not directly under NSRDS program management, also supply evaluated data relevant to this area of interest:

1. Title: JANAF Thermochemical Tables

   Location: Dow Thermal Research Laboratory, Midland, Michigan
   Director: H. Prophet

   Coverage: Thermodynamic properties in the solid, liquid, and/or ideal gaseous state over the temperature range of 0-6000°K. Covered are the following elements: Al, B, Ba, Be, Br, C, Ca, Cl, Co, Cs, F, Fe, H, Hg, I, K, Li, Mg, Mo, N, Na, Nb, O, P, Pb, S, Si, Sr, Ta, W, Zr, and e- and their simple compounds, principally those with the halogens, oxygen, and hydrogen. Properties given are heat capacity, entropy, Gibbs energy function, enthalpy (heat content), heat of formation, and Gibbs energy of formation for the ideal gas, liquid or solid state.

2. Title: Contributions to the Data on Theoretical Metallurgy

   Location: Thermodynamics Laboratory, Albany Metallurgy Research Center, Albany, Oregon
   Director: E. G. King; Project Director: A. D. Mah

   Coverage: The elements and their inorganic compounds of interest in metallurgical and ceramic operations. Included are oxides, halides, carbides, carbonates, sulfides, sulfates, nitrates, nitrides, and some intermetallic and interoxide compounds. Properties given include Gibbs energy, entropy, heat content (enthalpy), high and low temperature heat capacity, heat and free energy of formation and phase change, and vapor pressure.

3. Title: Thermochemistry for Steelmaking

   Location: Department of Metallurgy, Massachusetts Institute of Technology, Cambridge, Massachusetts
   Director: J. F. Elliott

   Coverage: Selected elements and compounds involved in the chemistry and technology of steelmaking. The compounds include: carbides, nitrides, oxides, phosphides, silicides, and sulfides. Binary and ternary iron alloys and solutions, complex oxide systems, and slags are also treated. The properties include: heat content (enthalpy) and temperature of phase changes; heat capacity; enthalpy, entropy and Gibbs energy function as appropriate.

B. ATOMIC AND MOLECULAR DATA

The NSRDS program for Atomic and Molecular Data places major emphasis on two elements. The first is preparation of data compilations on atomic and molecular spectroscopy, collision cross-section, ionization processes and related subjects. The second element is cooperative development and application of data standards, evaluation criteria, and compilation planning for several of the specific fields of molecular spectroscopy. Panels of outside advisors, including representatives of appropriate professional societies, are features of these latter efforts, which seek to coordinate and assist data compilation activities. The Joint Committee on Atomic and Molecular Physical Data is an important focal point for broad professional participation in such activities.

1. Title: Adjustments to Fundamental Constants

   Location: Electricity Division, NBS, Washington, D. C.
   Project Leader: Barry N. Taylor

   Description: This project provides for continuing overview of the latest accomplishments in the field of precision measurements and fundamental constants. The work is directed to new least-squares adjustments of the values for the constants as required by the state of the art. Under this project a quarterly preprint advisory service is maintained through the publication of "Preprints on Precision Measurement and Fundamental Constants (PPMFC)."

2. Title: Atomic Energy Levels Data Center

   Location: Optical Physics Division, NBS, Washington, D. C.
   Project Leader: W. C. Martin
   Address Inquiries to: Lucy Hagan

   Description: This data center maintains a current bibliography on atomic energy levels and spectra and compiles evaluated data in this area. A compilation of the energy levels of iron in all 26 ionization stages has just been completed, and a compilation of the levels of the lanthanide atoms and ions is at an advanced stage. A bibliography on atomic energy levels and spectra covering the period July 1971 through June 1974 will be published during FY 76.

3. Title: Transition Probabilities Data Center

   Location: Optical Physics Division, NBS, Washington, D. C.
   Project Leader: W. L. Wiese

   Description: The data center on atomic transition probabilities collects and catalogs all the literature containing numerical data on this atomic quantity. The data are critically evaluated and compiled in large tabulations, ordered by elements and stages of ionization. Bibliographies and tables of recommended data are the principal outputs of the center.

4. Title: Data Center on Atomic Line Shapes and Shifts

   Location: Optical Physics Division, NBS. Washington, D. C.
   Project Leader: L. J. Roszman

   Description: The data center on atomic line shapes and shifts collects and catalogs all literature related to these atomic quantities. Bibliographies and critical reviews of experimental and theoretical data are the principal output of the center.

5. Title: Electromagnetic Cross Section Compilations

Location: Center for Radiation Research, NBS, Washington, D. C.
Project Leader: J. H. Hubbell

Description: The project involves operation of an OSRD-sponsored "X-Ray and Ionizing Radiation Data Center" (formally "X-Ray Attenuation Coefficient Information Center") which provides standard reference data on the interactions of X-Rays, gamma-rays and charged particles with atoms and molecules and with bulk matter. The purpose is to provide information needed for the safe and efficient use of these radiations in nuclear energy technology, medicine, and national defense applications. Up to the present the work has been concentrated in the area of X-Ray cross sections; added emphasis is now being given to the compilation of charged particle cross sections and of radiation transport data for engineering applications.

6. Title: Atomic Collision Cross Section Information Center

Location: Laboratory Astrophysics Division, NBS, Boulder, Colorado
Project Leader: Earl Beaty

Description: The Atomic Collision Cross Section Information Center collects and evaluates data on low energy collisions between electrons, atoms, molecules and photons. Comprehensive annotated bibliographies of papers giving electron collision cross sections, photoabsorption and ionization cross sections, and electron-gas interactions are current and kept up to date. The total collection contains about 6,000 references. An extensive data bank, stored on magnetic tape, is updated and used to prepare critical data compilations and critical reviews. An extensive compilation of electron swarm data and a bibliography will be submitted for publication. A critical review of atomic electron affinities will be initiated. A critical compilation of electron collision cross sections for atomic hydrogen and the alkali metal atoms needed for modeling MHD plasmas will be started.

7. Title: Data Center for Atomic and Molecular Ionization Processes

Location: Physical Chemistry Division, NBS, Washington, D. C.
Project Leader: H. M. Rosenstock

Description: The activities of the Data Center consist of literature searching, abstracting, critical evaluation and dissemination of data on ionization and ion fragmentation thresholds and on heats of formation of gaseous ions.

8. Title: Diatomic Spectra Data

Location: Optical Physics Division, NBS, Washington, D. C.
Project Leader: Paul H. Krupenie

Description: This project provides for the collection, critical evaluation, and dissemination of spectral data for selected molecules of high interest. Current work centers on the preparation of a monograph compiling the spectroscopic data on the nitrogen molecule. As the principal constituent of air, nitrogen plays a significant role in atmospheric phenomena including aurorae and airglows. Nitrogen spectra are also important to a variety of laboratory experiments involving lasers, discharges, and afterglows. The monograph on nitrogen will be published in FY '76.

9. Title: Index to High Resolution Spectral Data

Location: Optical Physics Division, NBS, Washington, D. C.
Project Leader: Paul H. Krupenie

Description: This project provides for the compilation and dissemination of high resolution infrared spectral data for gases. The output of this project will be an index to high resolution measurements which will be useful for the application of lasers to many fields.

10. Title: Microwave Spectral Tables

Location: Optical Physics Division, NBS, Washington, D. C.
Project Leader: Frank J. Lovas

Description: This project provides a continuing data center for the collection, critical evaluation and dissemination of microwave spectral data for gases. The compilation of the microwave spectra of diatomic molecules has been completed and published. The next volume on triatomic molecules is under way. The review series on molecules of astrophysical interest now includes publications on H_2O, OCS, HCN, CO, CS, SiO, and SO, with HNCO nearing completion. CH_3CHO_3 will be initiated during FY '76. Reports concerning radio telescope searches providing unidentified lines or negative results are being distributed on a periodic basis.

11. Title: Fundamental Vibration Frequencies of Molecules

Location: Department of Physical Chemistry, University of Tokyo, Tokyo, Japan
Project Leader: T. Shimanouchi

Description: This project provides continuing preparation and publication of tables of data of the fundamental vibration frequencies of molecules. Spectroscopic measurements reported in the open literature are collected, selected, analyzed and evaluated to provide consistent and intercomparable data. Tables are published in sets (of about 50) bringing together data on molecules of similar structure and symmetry. Current efforts are directed to the preparation of a consolidated volume of tables, updating and bringing together material from the last four sets of tables.

12. Title: NMR Data Compilation

Location: Department of Chemistry, Texas A&M University, College Station, Texas
Project Leader: B. L. Shapiro

Description: This project is directed to the compilation, evaluation and publication of data derived from high-resolution proton NMR spectroscopy (chemical shifts and coupling constants) on aromatic molecules in which the proton is attached directly to an aromatic carbon atom.

13. Title: Vibrational Force Field Constants for Polyethylene

Location: Polymers Division, NBS, Washington, D. C.
Project Leader: D. H. Reneker

Description: Review of the previous efforts to describe the force field of polyethylene revealed inadequacy in the manner in which those force fields were formulated. Also, a large body of new data, principally in the low frequency Raman region, has been published since the most recent comprehensive review. Molecular vibrational data from the literature and from measurements made at NBS will be collected and used to obtain the best fit to theoretical dispersion curves of polyethylene crystals.

The following data center, not directly under NSRDS program management, also supplies evaluated data relevant to this area of interest:

Title: AP144-TRC Selected Spectral Data

Location: Thermodynamics Research Center, Texas A&M University, College Station, Texas

Director: B. J. Zwolinski

Coverage: Infrared, ultraviolet, mass Raman and nuclear magnetic resonance spectroscopic data on organic and inorganic compounds.

C. CHEMICAL KINETICS PROPERTIES DATA

This program deals primarily with rate constants of chemical reactions in the gaseous, liquid, and solid phases. Data center activities have focused on gas phase reaction rate constants and radiation chemical reaction data in gas and liquid phase. Individual data projects responsive to national problems have been emphasized. Some effort is being directed toward increasing activity in liquid phase kinetics data.

Programmatic advice and direction is supplied through close contact with leading kinetics experts and through NAS-NRC ad hoc advisory committees.

1. Title: Radiation Chemistry Data Center

Location: Radiation Laboratory, University of Notre Dame, Notre Dame, Indiana
Project Leader: Alberta Ross

Description: The Center's objectives are to compile, evaluate and disseminate reviews of data from radiation chemistry. The project has developed an automated literature reference file pertinent to radiation chemistry. In addition to maintaining a searchable file (over 22,000 papers since 1966), and the issuance of a bi-weekly current-awareness publication and some bibliographies, the Center prepares data compilations as input to critical reviews. Three critical reviews (on NH_3, N_2O and ethanol) have recently been published in the NSRDS-NBS series, and another (on methanol) has been submitted. Compilations of reaction rates of transients in solution are in press. Data reviews on electron mobility and G (free ions), additional compilations of rates of transients in solution, and collection of transient spectra (trapped and solvated electrons) are planned. (This Center is funded under a joint agreement between NBS and the Energy Research and Development Administration.)

2. Title: Chemical Kinetics Information Center

Location: Physical Chemistry Division, NBS, Washington, D. C.
Project Leader: David Garvin

Description: This Data Center abstracts and compiles chemical kinetic data from the literature. The Center has recently prepared and issued tables of rate data for use in atmospheric modelling, provided bibliographic services to the public, evaluated rate and photochemical data, coordinated preparation of text on the chemistry of the stratosphere and participated in international activities in the area of chemical kinetics.

D. SOLID STATE PROPERTIES

The activities in this program have emphasized selected solid state properties, principally optical, magnetic, surface, and transport data. Material coverage includes metals and alloys, organic and inorganic crystals, and special materials such as superconductors. A number of data centers compile and evaluate the data for publication. Individual projects in special areas of concern supplement the data center activities.

Programmatic liaison is maintained with related data centers sponsored by other governmental and non-governmental agencies. In some instances, jointly-sponsored programs are carried out. Advice and direction are provided by an NAS-NRC ad hoc committee of experts.

1. Title: Superconductive Materials Data Center

Location: General Electric, Schenectady, New York
Project Leader: B. W. Roberts

Description: The Superconductive Materials Data Center collects and disseminates the publicly known data on the basic physical properties of superconductive materials. The data include critical temperatures, critical magnetic field, crystallographic description, etc. The data are maintained on a keypunch card file. Previous publications included "Progress in Cryogenics" and a sequence of alternate year publication of NBS Technical Notes (No's. 408, 482, 724 and very recently, April 1974, No. 825). In addition, contributions of data listings have been made to the "Handbook of Chemistry and Physics," the "American Institute of Physics Handbook," and the "Handbook of Applied Engineering Science." Plans for 1975-76 call for the collation, condensation and critical evaluation of the accumulated data into one review.

2. Title: Cambridge Data Centre

Location: University of Cambridge, Cambridge, England
Project Leader: Olga Kennard

Description: The Cambridge Data Centre searches, extracts, compiles and stores crystal data from the world literature on organic compounds. In addition the Centre extracts information from the literature on inorganic compounds, intermetallics and minerals which it sends to the Single Crystal Data Center at NBS. The data on organic compounds are stored in a computerized file and include unit cell constants, densities and space group designation. These parameters serve as a basis for the identification and analytical determinations of such diverse material as petrochemicals, insecticides, drugs, biological compounds and others. The existence of this data file dissemination in selected form was instrumented to produce the publication of the Organic Compound volume of the third edition of "Crystal Data - Determinative Tables."

3. Title: Data Compilation - Crystal Data

Location: Inorganic Materials Division, NBS, Washington, D. C.
Project Leader: Helen M. Ondik

Description: The Crystal Data Center compiles and evaluates inorganic crystallographic data from the literature for dissemination to the scientific and technical community. With the third edition of Crystal Data Determinative Tables in print, the effort is aimed at preparing and publishing a series of supplements containing data from 1967 to date. Data for the first supplement is being compiled, the current file of punched cards containing about one-quarter to one-third of the expected total. During FY '76 the bulk of the entries for the first supplement (at least three-fourth of the total) should be in the processed file.

4. Title: Mossbauer Effect Data Index (MEDI)

Location: University of North Carolina, Asheville, North Carolina
Project Leader: John G. Stevens

Description: The literature involving Mossbauer effect measurements has grown steadily in recent years; it has application in such diverse areas as solid state physics, analytical chemistry, biophysics, etc. Annual publication of the Mossbauer Effect Data Index (MEDI) was initiated to provide workers with a single source of data and bibliographic reference thereby avoiding duplication of effort spent in searching the literature. The data include radioactive source, absorber employed, temperature, degree of shift, quadruple splitting, etc., the MEDI has been published annually starting with 1970, and the 1973 edition has just issued. Data for the 1974 Index are now being accumulated.

5. Title: Refractive Index Evaluation & Compilation

Location: Optical Physics Division, NBS, Washington, D. C.
Project Leader: Irving H. Malitson

Description: The project has been established to produce a compilation of critically evaluated refractive index data pertinent to laser, holographic and electro-optic systems. The work is a joint effort between NBS, the Research Materials Information Center (RMIC)-Oak Ridge National Laboratory, and the Thermophysical Properties Research Center (TPRD)-Purdue University. TPRC is compiling and evaluating halide laser window materials. NBS serves as an advisor and critical reviewer to the inputs of RMIC and TPRC. A trial evaluation of KCl and ZnSe has been completed. Critically evaluated data will form the basis for publication.

6. Title: Alloy Data Center

Location: Metallurgy Division, NBS, Washington, D. C.
Project Leader: Gesina C. Carter

Description: The Alloy Data Center (ADC) maintains complete and up-to-date reference files in the area of nuclear magnetic resonance (NMR) and includes a complete file on soft x-ray spectroscopy (SXS) papers up to 1973. In addition to these two areas, in which critical evaluation is carried out, the ADC covers a much broader scope of alloy physical properties. A general awareness is maintained of events in this broader area, which are related to NMR, SXS and other research carried out in the Alloy Physics Section.

7. Title: Diffusion in Metals Data Center

Location: Metallurgy Division, NBS, Washington, D. C.
Project Leader: J. R. Manning

Description: The project objective is the publication of standard reference data monographs which review and critically evaluate data on diffusion in metals and their alloys. Papers from the technical literature are systematically collected and classified according to the alloy systems on which they report diffusion data. More than 14,000 papers are currently in our files. Diffusion monographs for alloy systems important in technology are being produced, starting with diffusion in copper and copper alloys. The overall aim of this project is to provide a comprehensive source of evaluated diffusion data, including data on the more complex alloy systems. Three evaluated data compilations have been published.

8. Title: Thermal Expansion Compilation

Location: Inorganic Materials Division, NBS, Washington, D. C.
Project Leader: Richard K. Kirby

Description: The thermal expansion compilation effort is aimed at preparing critically evaluated data on elements and selected compounds for publication in the TPRC Data Series.

The following data centers, not directly under NSRDS program management, also supply evaluated data relevant to this area of interest:

1. Title: Phase Diagrams for Ceramists

Location: Inorganic Materials Division, NBS, Washington, D. C.
Director: Lawrence P. Cook

Coverage: Systems of special interest to ceramists: metal-oxygen and metal oxide systems (including Si), systems with oxygen-containing radical systems containing halides, sulfides, alone and with other substances, systems of water with metal oxide and miscellaneous substances. Phase diagrams for one-, two-, three-, component systems as a function of temperature.

2. Title: Rare Earth Information Center

Location: Iowa State University, Ames, Iowa
Director: Karl A. Gschneidner, Jr.

Coverage: Physical metallurgy and solid state physics of rare earth metals and their alloys; analytical, physical chemical, toxicity data on rare earth elements and compounds.

E. NUCLEAR DATA

The former Atomic Energy Commission, now the Energy Research and Development Administration, has supported extensive activities on neutron cross sections and other nuclear data. The Office of Standard Reference Data maintains close liaison with this work, and in some cases has provided support for data centers jointly with ERDA. The present emphasis of OSRD support is on photonuclear data.

1. Title: Table of Isotopes Project

   Location: Lawrence Radiation Laboratory, University of California, Berkeley, California
   Project Leader: C. Michael Lederer

   Description: The project publishes periodic editions of the Table of Isotopes, a compact, comprehensive compilation of evaluated data on radioactive decay and nuclear level properties for all nuclei. Experimental data covered include halflives of ground and excited states, decay modes and branching, masses and Q-values, natural abundances, nuclear spins and moments, thermal neutron cross sections, means of production, detailed data on all types of radiation (beta, alpha, proton, neutron and electromagnetic radiation, including γ-rays, X-rays and conversion electrons), and nuclear level schemes. Level schemes include data derived from both radioactive decay and nuclear reactions. Since 1971, extensive automation of the data handling has been under development in order (1) to cope with the greatly accelerated generation of new data, (2) to enable the publication of subsequent editions at shorter intervals, and (3) to permit the publication of secondary compilations and the creation of computerized data services of particular utility to scientists who need nuclear data for practical applications. In FY 1975, approximately two thirds of the data intended for the 7th edition have been evaluated.

2. Title: Berkeley Particle Data Center

   Location: Lawrence Berkeley Laboratory, University of California, Berkeley, California
   Project Leader: Arthur H. Rosenfeld

   Description: This data center collects, compiles, indexes, evaluates, and disseminates data on the properties and interactions of elementary particles, including protons, leptons, mesons, and baryons. The Center publishes the annual "Review of Particle Properties," a critical examination and summary of the properties of elementary particles. It also produces, at irregular intervals, compilation reports of cross sections and other measured quantities for particle interactions. A literature file is maintained, and data extracted from the literature are stored partly in a card image file and partly in a more sophisticated data file. An index of all experimental particle physics documents is being prepared from the latter.

3. Title: Compilation and Evaluation of Photonuclear Data

   Location: Nuclear Sciences Division, NBS, Washington, D. C.
   Project Leader: E. G. Fuller

   Description: This data center systematically abstracts, collects, and indexes data from the published literature; maintains a library of digitized cross section data; and serves as an information center for the field of photonuclear physics. A literature file from 1955 contains over 2000 journal papers; the data abstract files contain information on over 4800 separate measurements, and the digital library contains data for over 700 cross section curves. A comprehensive compilation of evaluated photonuclear reactions cross section data is being prepared. This will be published in three sections, each covering a section of the periodic table.

4. Title: Tables of Nuclear Spins and Moments

Location: Office of Standard Reference Data, NBS, Washington, D. C.
Project Leader: G. H. Fuller

Description: The pertinent literature on nuclear spins and moments is being compiled, evaluated and tabulated for publication. The new set of tables represent an updated version of the tables published by V. H. Cohen and G. H. Fuller in Nuclear Data Tables, A5, No. 5-6 (1969). The previous data has been incorporated into the new tables as appropriate.

The following data centers, not directly under NSRDS program management, also supply evaluated data relevant to this area of interest:

1. Title: Nuclear Data Project

Location: Oak Ridge National Laboratory, P. O. Box X, Oak Ridge, Tennessee
Director: Daniel J. Horen

Coverage: Data on the physics of nuclear structure and other nuclear properties. Emphasis is placed on evaluated energy level data for nuclides of A>40.

2. Title: National Neutron Cross Secton Center

Location: Brookhaven National Laboratory, Upton, New York
Director: S. Pearlstein

Coverage: Data on neutron-induced nuclear reactions and related parameters, consisting mainly of energy and angle dependent cross sections for use in reactor design, neutronics calculations and nuclear physics studies.

3. Title: Physical Data Group

Location: Lawrence Radiation Laboratory, University of California, Livermore, California
Director: Robert J. Howerton

Coverage: Neutron and photon cross section data required for weapon effects, shielding and reactor calculations; static and dynamic parameters of critical assemblies and bulk experiments relating to neutron multiplication and transport.

F. MECHANICAL PROPERTIES

Limited funds have so far restricted activities in the mechanical properties area to one data evaluation project concerned with elastic properties of metals and alloys, and the Surveys of Data Sources described in Section II above.

1. Title: Elastic Constant Data for Metals and Alloys

Location: Cryogenics Division, NBS, Boulder, Colorado
Project Leader: R. P. Reed
Address Inquiries to: H. Ledbetter

Description: Elastic properties data for materials that are of scientific or technological interest because of their relationship to the interatomic potential in solids and, consequently, to a wide variety of solid-state phenomena. Technologically, elastic constants are essential design parameters in any mechanically stressed component--pressure vessels, ship hulls, rotating machinery, etc.

The first review in this series covered Iron, Nickel, and Iron-Nickel Alloys (J. Phys. Chem. Ref. Data, 2 (1974), 531-618).

During FY '75, a paper on the elastic properties of copper was published (J. Phys. Chem. Ref. Data, 3, (1974, 897-935). Also, a note on the elastic constants of polycrystals was published (Phys. Status Solidi, 2, 26 (1974), K67-70). A manuscript on the elastic properties of zinc is in preparation.

During FY '76, it is expected that reviews on copper-zinc alloys and on aluminum will be forthcoming.

2. Title: Critical Surveys of Data Sources

Location: Battelle Columbus Laboratories, Columbus Ohio, and General Electric Company, Schenectady, New York
Project Leaders: J. F. Lynch (Battelle) and J. H. Westbrook (General Electric)

Description: A series of surveys covering sources of numerical data covering selected materials and properties is being prepared. The emphasis is on coverage of commercial materials (those used in construction and manufacturing), for which the sources of information are numerous and of diverse character, making it extremely difficult for a practicing engineer or materials scientist to locate the best source of data for his particular needs.

Current Status:

a. Mechanical Properties of Metals, by R. B. Gavert, R. L. Moore, and J. H. Westbrook, Engineering Consulting Service, General Electric Company. Published as NBS SP 396-1, September 1974.

b. Properties of Ceramics.

Principal Investigator: James F. Lynch
Location: Metals and Ceramics Information Center, Battelle Columbus Laboratories

Manuscript and review by task force formed by the American Ceramic Society completed. Publication expected by mid-1975.

The Publications Committee of the National Association of Corrosion Engineers has agreed to serve as a review panel for the survey. Completion is expected by mid-1975.

c. Electrical and Magnetic Properties of Metals.

Principal Investigator: J. H. Westbrook
Location: Materials Information Services, General Electric Company

Initial manuscript and review by task force from the Magnetics Society of IEEE and ASTM completed.

d. Corrosion Data.

Principal Investigator: Ronald B. Diegle
Location: Corrosion and Electrochemical Technology Section, Battelle Columbus Laboratories

APPENDIX IA

FEDERAL COUNCIL FOR SCIENCE AND TECHNOLOGY
COMMITTEE ON SCIENTIFIC INFORMATION
28 May 1963

Federal Policy on National Standard Reference Data System

There will be established a National Standard Reference Data System (NSRDS) to provide on a national basis critically evaluated data in the physical sciences. The NSRDS will consist of a National Standard Reference Data Center (NSRDC) at the National Bureau of Standards and such other Standard Reference Data Centers as may be required.

The National Bureau of Standards will be charged with the administration of the National Standard Reference Data System. This assignment will include the establishment of standards of quality, methodology including machine processing formats, and such other functions as are required to ensure the compatibility of all units of the NSRDS.

The National Bureau of Standards will be charged with funding and administering the National Standard Reference Data Center. This Center will be an identifiable part of the National Scientific and Technical Information System (NSTIS).

Standard Reference Data Centers covering certain specific areas of effort may be established by or be assigned to the various Departments and Agencies in accordance with their specific desires and capabilities. Such Centers will be financed and administered by the Department to which assigned but will meet the quality standards and other requirements of the NSRDS. Such Centers will be included as identifiable components of the NSTIS.

The NSRDS may also include Standard Reference Data Centers at universities, research institutes, and other appropriate non-Government activities. To be included in the NSRDS, such Centers will meet the quality standards and other requirements of the NSRDS and will be included as identifiable components of the NSTIS.

There will be an Advisory Board to review and recommend policy relative to the operation of the NSRDS. It will include among others, representation from the National Academy of Sciences, National Science Foundation, Federal Agencies engaged in research and development, and such other representatives of the scientific and technical community as the Director of the National Bureau of Standards may determine.

In establishing the NSRDS, the intent is to provide an articulated system of Centers and activities under such coordination and direction as to ensure an output meeting quality standards for national reference data in the physical sciences. The establishment of the System should not be construed as preventing the establishment of such Federal or Departmental Data Systems as are required for the collection of raw or evaluated data to serve engineering or operating needs of the Federal Government or various Federal agencies.

APPENDIX IB

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

Appendix II

Publications List

Publications in
The Journal of Physical and Chemical
Reference Data

1. *Gaseous Diffusion Coefficients* - T.R. Marrero and E.A. Mason, Vol. 1, No. 1 (1972). $7.00
2. *Selected Values of Critical Supersaturation for Nucleation of Liquids from the Vapor* - G.M. Pound, Vol. 1, No. 1 (1972). $3.00
3. *Selected Values of Evaporation and Condensation Coefficients of Simple Substances* - G.M. Pound, Vol. 1, No. 1 (1972). $3.00
4. *Atlas of the Observed Absorption Spectrum of Carbon Monoxide between 1060 and 1900 Å* - S.G. Tilford and J.D. Simmons, Vol. 1, No. 1 (1972). $4.50
5. *Tables of Molecular Vibrational Frequencies, Part 5* - T. Shimanouchi, Vol. 1, No. 1 (1972). $4.00
6. *Selected Values of Heats of Combustion and Heats of Formation of Organic Compounds Containing the Elements C,H,N,O,P, and S* - Eugene S. Domalski, Vol. 1, No. 2 (1972). $5.00
7. *Thermal Conductivity of the Elements* - C.Y. Ho, R.W. Powell, and P.E. Liley, Vol. 1, No. 2 (1972). $7.50
8. *The Spectrum of Molecular Oxygen* - Paul H. Krupenie, Vol. 1, No. 2 (1972). $6.50
9. *A Critical Review of the Gas-Phase Reaction Kinetics of the Hydroxyl Radical* - W.E. Wilson,Jr., Vol. 1, No. 2 (1972). $4.50
10. *Molten Salts: Volume 3, Nitrates, Nitrites, and Mixtures, Electrical Conductance, Density, Viscosity, and Surface Tension Data* - G.J. Janz, Ursula Krebs, H.F. Siegenthaler and R.P.T. Tomkins, Vol. 1, No. 3 (1972). $8.50
11. *High Temperature Properties and Decomposition of Inorganic Salts - Part 3. Nitrates and Nitrites* - Kurt H. Stern, Vol. 1, No. 3 (1972). $4.00
12. *High-Pressure Calibration: A Critical Review* - D.L. Decker, W.A. Bassett, L. Merrill, H.T. Hall, and J.D. Barnett, Vol. 1, No. 3 (1972). $5.00
13. *The Surface Tension of Pure Liquid Compounds* - Joseph J. Jasper, Vol. 1, No. 4 (1972). $8.50
14. *Microwave Spectra of Molecules of Astrophysical Interest, I. Formaldehyde, Formamide, and Thioformaldehyde* - Donald R. Johnson, Frank J. Lovas, and William H. Kirchhoff, Vol. 1, No. 4 (1972). $4.50
15. *Osmotic Coefficients and Mean Activity Coefficients of Uni-univalent Electrolytes in Water at 25 C* - Walter J. Hamer and Yung Chi Wu, Vol. 1, No. 4 (1972). $5.00
16. *The Viscosity and Thermal Conductivity Coefficients of Gaseous and Liquid Fluorine* - H.J.M. Hanley and R. Prydz, Vol. 1, No. 4 (1972). $3.00
17. *Microwave Spectra of Molecules of Astrophysical Interest, II. Methylenimine* - William H. Kirchhoff, Donald R. Johnson, and Frank J. Lovas, Vol. 2, No. 1 (1973). $3.00
18. *Analysis of Specific Heat Data in the Critical Region of Magnetic Solids* - F.J. Cook, Vol. 2, No. 1 (1973). $3.00
19. *Evaluated Chemical Kinetic Rate Constants for Various Gas Phase Reactions* - Keith Schofield, Vol. 2, No. 1 (1973). $5.00
20. *Atomic Transition Probabilities for Forbidden Lines of the Iron Group Elements. (A Critical Data Compilation for Selected Lines)* - M.W. Smith and W.L. Wiese, Vol. 2, No. 1 (1973). $4.50
21. *Tables of Molecular Vibrational Frequencies, Part 6* - T. Shimanouchi, Vol. 2, No. 1 (1973). $4.50
22. *Compilation of Energ/ Band Gaps in Elemental and Binary Compound Semiconductors and Insulators* - W.H. Strehlow and E.L. Cook, Vol. 2, No. 1 (1973). $4.50
23. *Microwave Spectra of Molecules of Astrophysical Interest, III. Methanol* - R.M. Lees, F.J. Lovas, W.H. Kirchhoff, and D.R. Johnson, Vol. 2, No. 2 (1973). $3.00
24. *Microwave Spectra of Molecules of Astrophysical Interest, IV. Hydrogen Sulfide* - Paul Helminger, Frank C. DeLucia and William H. Kirchhoff, Vol. 2, No. 2 (1973). $3.00

25. *Tables of Molecular Vibrational Frequencies, Part 7* - T. Shimanouchi, Vol. 2, No. 2 (1973). $4.00
26. *Energy Levels of Neutral Helium (^4He I)* - W.C. Martin, Vol. 2, No. 2 (1973). $3.00
27. *Survey of Photochemical and Rate Data for Twenty-eight Reactions of Interest in Atmospheric Chemistry* - R.F. Hampson, W.Braun, R.L. Brown, D. Garvin, J.T. Herron, R.E. Huie, M.J. Kurylo, A.H. Laufer, J. D. McKinley, H. Okabe, M.D. Scheer, W. Tsang, and D.H. Stedman, Vol. 2, No. 2 (1973). $4.50
28. *Compilation of the Static Dielectric Constant of Inorganic Solids* - K.F. Young and H.P.R. Frederikse, Vol. 2, No. 2 (1973). $6.00
29. *Soft X-Ray Emission Spectra of Metallic Solids: Critical Review of Selected Systems* - A.J. McAlister, R.C. Dobbyn, J.R. Cuthill, and M.L. Williams, Vol. 2, No. 2 (1973). $3.00
30. *Ideal Gas Thermodynamic Properties of Ethane and Propane* - J. Chao, R.C. Wilhoit, and B.J. Zwolinski, Vol. 2, No. 2 (1973). $3.00
31. *An Analysis of Coexistence Curve Data for Several Binary Liquid Mixtures Near Their Critical Points* - A. Stein and G.F. Allen, Vol. 2, No. 3 (1973). $4.00
32. *Rate Constants for the Reactions of Atomic Oxygen (O^3P) With Organic Compounds in the Gas Phase* - John T. Herron and Robert E. Huie, Vol. 2, No. 3 (1973). $5.00
33. *First Spectra of Neon, Argon, and Xenon 136 in the 1.2-4.0 μm Region* - Curtis J. Humphreys, Vol. 2, No. 3 (1973). $3.00
34. *Elastic Properties of Metals and Alloys, I. Iron, Nickel, and Iron-Nickel Alloys* - H.M. Ledbetter and R.P. Reed, Vol. 2, No. 3 (1973). $6.00
35. *The Viscosity and Thermal Conductivity Coefficients of Dilute Argon, Krypton, and Xenon* - H.J.M. Hanley, Vol. 2, No. 3 (1973). $4.00
36. *Diffusion in Copper and Copper Alloys, Part I. Volume and Surface Self-Diffusion in Copper* - Daniel B. Butrymowicz, John R. Manning, and Michael E. Read, Vol. 2, No. 3 (1973). $3.00
37. *The 1973 Least-Squares Adjustment of the Fundamental Constants* - E. Richard Cohen and B.N. Taylor, Vol. 2, No. 4 (1973). $5.50
38. *The Viscosity and Thermal Conductivity Coefficients of Dilute Nitrogen and Oxygen* - H.J.M. Hanley and James F. Ely, Vol. 2, No. 4 (1973). $4.00
39. *Thermodynamic Properties of Nitrogen Including Liquid and Vapor Phases from 63 K to 2000 K with Pressures to 10,000 Bar* - Richard T. Jacobsen and Richard B. Stewart, Vol. 2, No. 4 (1973). $8.50
40. *Thermodynamic Properties of Helium 4 from 2 to 1500 K at Pressures to 10^8Pa* - Robert D. McCarty, Vol. 2, No. 4 (1973). $7.00
41. *Molten Salts: Volume 4, Part 1, Fluorides and Mixtures, Electrical Conductance, Density, Viscosity, and Surface Tension Data* - G.J. Janz, G.L. Gardner, Ursula Krebs, and R.P.T. Tomkins, Vol. 3, No. 1 (1974). $7.00
42. *Ideal Gas Thermodynamic Properties of Eight Chloro- and Fluoromethanes* - A.S. Rodgers, J. Chao, R.C. Wilhoit, and B.J. Zwolinski, Vol. 3, No. 1 (1974). $4.00
43. *Ideal Gas Thermodynamic Properties of Six Chloroethanes* - J. Chao, A.S. Rodgers, R.C. Wilhoit, and B.J. Zwolinski, Vol. 3, No. 1 (1974). $4.00
44. *Critical Analysis of Heat-Capacity Data and Evaluation of Thermodynamic Properties of Ruthenium, Rhodium, Palladium, Iridium, and Platinum from 0 to 300 K. A Survey of the Literature Data on Osmium* - George T. Furukawa, Martin L. Reilly, and John S. Gallagher, Vol. 3, No. 1 (1974). $4.50
45. *Microwave Spectra of Molecules of Astrophysical Interest, V. Water Vapor* - Frank C. DeLucia, Paul Helminger, and William H. Kirchhoff, Vol. 3, No. 1 (1974). $3.00
46. *Microwave Spectra of Molecules of Astrophysical Interest, VI. Carbonyl Sulfide and Hydrogen Cyanide* - Arthur G. Maki, Vol. 3, No. 1 (1974). $4.00
47. *Microwave Spectra of Molecules of Astrophysical Interest, VII. Carbon Monoxide, Carbon Monosulfide, and Silicon Monoxide* - Frank J. Lovas and Paul H. Krupenie, Vol. 3, No. 1 (1974). $3.00
48. *Microwave Spectra of Molecules of Astrophysical Interest VIII Sulfur Monoxide* - Eberhard Tiemann, Vol.3, No. 1 (1974). $3.00
49. *Tables of Molecular Vibrational Frequencies, Part 8* - T. Shimanouchi, Vol. 3, No. 1 (1974). $4.50
50. *JANAF Thermochemical Tables, 1974 Supplement* - M.W. Chase, J.L. Curnutt, A.T. Hu, H. Prophet, A.N. Syverud, and L.C. Walker, Vol. 3, No. 2 (1974). $8.50
51. *High Temperature Properties and*

Decomposition of Inorganic Salts - Part 4. Oxy-Salts of the Halogens - Kurt H. Stern, Vol. 3. No. 2 (1974). $4.50

52. *Diffusion in Copper and Copper Alloys, Part II. Copper-Silver and Copper-Gold Systems* - Daniel B. Butrymowicz, John R. Manning, and Michael E. Read, Vol. 3, No. 2 (1974). $5.50
53. *Microwave Spectral Tables, I. Diatomic Molecules* - Frank J. Lovas and Eberhard Tiemann, Vol. 3, No. 3 (1974). $8.50
54. *Ground Levels and Ionization Potentials for Lanthanide and Actinide Atoms and Ions* - W.C. Martin, Lucy Hagan, Joseph Reader, and Jack Sugar, Vol. 3, No. 3 (1974). $3.00
55. *Behavior of the Elements at High Pressure* - John Francis Cannon, Vol. 3, No. 3 (1974). $4.50
56. *Reference Wavelengths from Atomic Spectra in the Range 15A to 25000A* - Victor Kaufman and Bengt Edlen, Vol. 3, No.4 (1974). $5.50
57. *Elastic Properties of Metals and Alloys, II. Copper* - H.M. Ledbetter and E.R. Naimon, Vol. 3, No. 4 (1974). $4.50
58. *Critical Review of Hydrogen Atom Transfer Reactions in the Liquid Phases* - D.G. Hendry, T. Mill, J.A. Howard, L. Piszkiewicz, and H.K. Eigenmann, Vol. 3, No. 4 (1974). $4.50
59. *The Viscosity and Thermal Conductivity Coefficients for Dense Gaseous and Liquid Argon, Krypton, Xenon, Nitrogen, and Oxygen*- H.J.M. Hanley, R.D. McCarty, and W.N. Haynes, Vol. 3, No. 4 (1974). $4.50
60. *JANAF Thermochemical Tables, 1975 Supplement* - M.W. Chase, J.L. Curnutt, H.Prophet, R.A. McDonald, and A.N. Syverud, Vol. 4, No. 1 (1975). $8.50
61. *Diffusion in Copper and Copper Alloys, Part III. Diffusion in Systems Involving Elements of the Groups IA, IIA, IIIB, IVB, VB, VIB, and VIIB* - Daniel B. Butrymowicz, John R. Manning, and Michael E. Read, Vol. 4, No. 1 (1975). $6.00
62. *Ideal Gas Thermodynamic Properties of Ethylene and Propylene* - Jing Chao and Bruno J. Zwolinski, Vol.4, No. 1 (1975). $3.00

Supplements to the Journal of Physical and Chemical Reference Data**

Physical and Thermodynamic Properties of Aliphatic Alcohols - R.C. Wilhoit and B.J. Zwolinski, Vol. 2 Supplement 1, 420 pp. (1973). Hardcover: $33.00; Softcover: members $10.00; non-members $30.00

Thermal Conductivity of the Elements: A Comprehensive Review - C.Y. Ho, R.W. Powell, and P.E. Liley, Vol. 3, Supplement 1, 796 pp. (1974). Hardcover: $60.00; Softcover: members $55.00, non-members $60.00

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Publications in the National Standard Reference Data Series

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NBS-114A (REV. 7-73)

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET	1. PUBLICATION OR REPORT NO. NBS TN-881	2. Gov't Accession No.	3. Recipient's Accession No.

4. TITLE AND SUBTITLE

Critical Evaluation of Data in the Physical Sciences -- A Status Report on the National Standard Reference Data System, April 1975

5. Publication Date: September 1975

6. Performing Organization Code

7. AUTHOR(S)
Stephen A. Rossmassler, Editor

8. Performing Organ. Report No.

9. PERFORMING ORGANIZATION NAME AND ADDRESS

NATIONAL BUREAU OF STANDARDS
DEPARTMENT OF COMMERCE
WASHINGTON, D.C. 20234

10. Project/Task/Work Unit No. 1510101

11. Contract/Grant No.

12. Sponsoring Organization Name and Complete Address *(Street, City, State, ZIP)*

Same as Item 9.

13. Type of Report & Period Covered

14. Sponsoring Agency Code

15. SUPPLEMENTARY NOTES

Library of Congress Catalog Card Number: 75-600066

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17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)* Atomic and molecular data; chemical kinetics; colloid and surface properties; mechanical properties; nuclear data; standard reference data; solid state data; thermodynamic data, transport properties.

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19. SECURITY CLASS (THIS REPORT)	21. NO. OF PAGES
UNCLASSIFIED	53
20. SECURITY CLASS (THIS PAGE)	22. Price
UNCLASSIFIED	$1.10

USCOMM-DC 29042-P74

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