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Technical Activities 1983 Office of Standard Reference Data

S. P. Fivozinsky, Editor

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards
National Measurement Laboratory
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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

ABSTRACT

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

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1983.

Key words: data compilation; energy and environmental data, evaluated data; materials data; standard reference data; technical activities 1983; thermochemical and thermophysical data

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INTRODUCTION

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

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

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

The Office of Standard Reference Data monitors and coordinates the work of the various data centers and specialized projects which collectively make up the NSRDS. These projects are located in the technical divisions of NBS and in universities, industrial laboratories, and other Government laboratories. Close association between data evaluation projects and relevant experimental research programs helps provide the critical judgment which is essential to assure the reliability of the final output.

*See Appendix G.

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

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

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

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

Appropriate publications of technical societies and commercial publishers.

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

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

OSRD COOPERATIVE ACTIVITIES

Important to the success of the Standard Reference Data Program are the ability to be aware of data requirements in the U.S. technical community, and the assistance of that community in accomplishing the job of providing needed data.

As a result, the Standard Reference Data Program carries out much of its work in collaboration with industrial and professional groups. These cooperative activities provide considerable assistance-in-kind to the Program as well as highly effective routes for the dissemination of needed databases.

This section of the Annual Report describes OSRD's major cooperative activities. Through some of these arrangements we also bring outside scientists to work at NBS, thus taking advantage of an expertise which may not exist in the Data Centers.

JOINT NUMERICAL DATA PUBLICATION PROGRAM WITH THE AMERICAN CHEMICAL SOCIETY AND THE AMERICAN INSTITUTE OF PHYSICS

In 1972, an agreement was reached between the NBS Office of Standard Reference Data (OSRD), the American Chemical Society (ACS), and the American Institute of Physics (AIP) for the publication of the Journal of Physical and Chemical Reference Data (JPCRD). The Journal, which is now in its eleventh year of publication, is the major printed output channel for the National Standard Reference Data System (NSRDS).

The Journal presents compilations of physical and chemical property data which have been critically evaluated by scientists who are knowledgeable in the pertinent field of research. However, it is not simply a collection of data tables. Its basic philosophy is that all compilations should be fully documented as to the original source of the measurement data and the criteria used to select and evaluate these data. Articles in the Journal also may take the form of critical reviews which discuss experimental error sources and assessments of the overall reliability of data in a particular field. Such reviews serve to point out state-of-the-art experimental technology and gaps in available information.

The American Chemical Society handles promotion and subscriptions to the Journal as well as sales of bound offprints of articles, a unique service of JPCRD. The American Institute of Physics carries out composition, printing, and mailing, while the National Bureau of Standards provides technical and editorial control. The Journal of Physical and Chemical Reference Data is the only scientific journal listed as both an ACS and AIP publication.

The participation of the ACS and the AIP in sponsoring this effort and actively disseminating the results to their membership gives recognition to the importance which professional societies attach to this endeavor.

AMERICAN SOCIETY FOR METALS/NBS PHASE DIAGRAM PROGRAM

The American Society for Metals/National Bureau of Standards (ASM/NBS) joint program on alloy phase diagrams has been active since 1978. Under this program, phase diagrams for binary and higher-order alloys are being evaluated, and recommended phase information is entered into a computerized database.

The project is well on the way to meeting its goal of creating a comprehensive set of reference phase diagrams which will meet the needs of materials scientists in industry, universities, and government.

The phase diagrams are evaluated by experts in their fields (referred to as category editors) who are selected by oversight committees. Each category editor is responsible for evaluating alloy phase diagrams for one or more assigned elements (e.g., aluminum). ASM provides computerized bibliographic references as well as hard copies of the pertinent literature to the category editors. When completed, the evaluations are rigorously reviewed under supervision of NBS. Upon acceptance of an evaluation, the graphical and numeric data are entered into a computerized database. In addition, the text and the computer-drawn phase diagrams are published in the joint ASM/NBS "Bulletin of Alloy Phase Diagrams."

NBS is responsible for assuring the technical accuracy of the data and setting up a prototype database. To do this, NBS has committed resources in the Metallurgy Division of the Center for Materials Science, in the Office of Standard Reference Data, and in the Mathematical Analysis Division of the Center for Applied Mathematics. The Alloy Phase Diagram Data Center in the Center for Materials Science is responsible for the NBS work. The data center also houses the category editors of the titanium, aluminum, and iron binary alloy systems. In addition, through the Office of Standard Reference Data and the Center for Materials Science, NBS provides funding for several other category editors.

The evaluation of a phase diagram is performed by understanding the original data and resolving any discrepancies. The phase stability described by the phase diagram is completely governed by the thermodynamics of the phases. Hence, a suitable thermodynamic model is used as an evaluation tool. In addition to providing much needed information about the equilibrium of phases, the thermodynamic model also provides information on metastable phases. The NBS Alloy Phase Diagram Data Center is developing and refining computerized thermodynamic models to accurately predict phase diagrams. The editors at NBS are working closely with internationally known scientists and other category editors to perfect this thermodynamic model and to make it an integral part of each evaluation effort.

INDUSTRY/NBS CERAMIC PHASE DIAGRAM SERVICES

In December 1982, the American Ceramic Society (ACerS) and NBS signed a three-year agreement that formally institutes a joint program to provide improved evaluated ceramic phase diagrams and related data to better serve the $50 billion-a-year ceramic industry.

Under the agreement, NBS, through the Phase Diagrams for Ceramists Data Center in the Inorganic Materials Division, Center for Materials Science, is responsible for overall guidance on the technical aspects and reliability of the data evaluations. The data center will provide coordination with other phase diagram compilation centers, compile evaluated phase equilibria data, and maintain a bibliographic data bank.

The agreement calls for ACerS to develop program and funding support from industry, government, and foundation sources and to publish and market "Phase

Diagrams for Ceramists" and associated publications. The evaluated data will be published and disseminated through the National Standard Reference Data System and ACerS channels.

ACerS also has agreed to sponsor a research associate program at NBS to help compile evaluated ceramic equilibria data and other associated data in both hard copy and computer-retrievable form. This will include compilations of evaluated binary and higher-order diagrams and related data in a form which enables retrieval and display in alphanumeric and/or graphic form. Currently, ceramic phase diagrams are available only in hard copy.

NATIONAL ASSOCIATION OF CORROSION ENGINEERS/NBS JOINT PROGRAM

The National Association of Corrosion Engineers (NACE) and NBS have set up a joint program to provide evaluated corrosion data on alloys and other materials. This program will give industry and others critically needed data for the design of products that are susceptible to the effects of corrosion. Corrosion cost the United States an estimated $126 billion in 1982, and this new cooperative program is aimed at reducing these costs by better utilization of materials and application of good corrosion-prevention practices.

The NACE/NBS program is designed first to develop criteria for evaluating different types of corrosion data, then to proceed with the actual evaluation. Through its Data Program Committee, NACE has agreed to help raise financial support from industry and to work with NBS to define the priorities and scope of the individual projects. The evaluated data resulting from the program will be distributed through new and traditional NACE publications as well as by computerized databases.

NBS, through the combined efforts of the Metallurgy Division of the Center for Materials Science and the Office of Standard Reference Data, has established a Corrosion Data Center. The NBS data center will be responsible for overall guidance of the technical aspects of the program and will assure reliability of the data evaluations. Evaluated data made available to the users will be part of the National Standard Reference Data System.

Several pilot projects will constitute the initial phase of this program. One will focus on corrosion-rate data for stainless steels in aqueous chloride solutions; another on atmospheric corrosion-rate data for structural alloys. The emphasis will be not only on the data themselves but also on how to evaluate these types of data.

NBS also plans to develop computer software to store and evaluate corrosion data. The first effort along these lines will be to develop software to generate potential-pH diagrams, also called stability diagrams. These provide basic information for determining the chemical, electrochemical, and corrosion properties of materials.

Both NACE and NBS view these projects as the beginning of a long-term effort to improve the quality of corrosion data and therefore to reduce the effects of corrosion.

JOINT NBS/AMERICAN INSTITUTE OF CHEMICAL ENGINEERS - INDUSTRY COOPERATIVE PROGRAM FOR EVALUATED NUMERICAL DATA

The Design Institute for Physical Properties Data (DIPPR) is a collaborative project involving NBS, the American Institute of Chemical Engineers and some 40 odd industrial organizations. Its purpose is to provide reference data for the chemical industry by critical evaluation and by experimental measurement.

DIPPR was founded in 1979. Administratively, it is an activity of the American Institute of Chemical Engineers. Interested organizations become members of DIPPR by paying yearly dues on a graduated scale. These dues cover the administrative costs of DIPPR. Interested organizations can also support any of the projects of DIPPR by paying yearly fees which depend on the size of the organization, the size of the project and the number of supporters of the project. At present, there are 6 projects: three involving the critical evaluation of data and three experimental measurements. An additional experimental project has been completed. Organizations supporting DIPPR include companies which manufacture chemical or petrochemicals, process and plant designers, and organizations which provide a variety of services to the chemical industry.

DIPPR projects are carried out by contract under the direction of an advisory committee selected by the industrial supporters. Reports are available to sponsors when written and are published in the open literature after one year. Products include research papers, data tables, data books, and data tapes.

NBS, through the Office of Standard Reference Data, played an active role in helping the industry get DIPPR started and cooperates with it in a number of ways which are spelled out in a research agreement between the two organizations. These include direct support of DIPPR projects by OSRD, and carrying out of work for DIPPR at NBS.

Provision of critically evaluated reference data to the chemical industry is a major goal of DIPPR and of OSRD; the programs of the two organizations complement and enhance one another. NBS staff serve on a variety of DIPPR technical and administrative committees in order to maintain close coordination between the two programs.

STANDARD REFERENCE DATA DISSEMINATED THROUGH AGREEMENT WITH THE JOINT COMMITTEE FOR POWDER DIFFRACTION STANDARDS - INTERNATIONAL CENTRE FOR DIFFRACTION DATA

A new cooperative effort has been established by the Office of Standard Reference Data (OSRD) and the Joint Committee for Powder Diffraction Standards-International Centre for Diffraction Data (JCPDS-ICDD) for the collection and dissemination of evaluated crystallographic diffraction data to the scientific and technical community. Under the agreement, JCPDS-ICDD will distribute NBS crystallographic databases in machine-readable form and as separate publications, and will assist the NBS Crystal Data Center in collecting and evaluating data for use in building and maintaining the computer databases.

The first NBS database JCPDS-ICDD will distribute is the NBS Crystal Data Identification File, which contains chemical and crystallographic information

on more than 60,000 organic, inorganic, and metallic substances. The data contained in this file can be used to identify uniquely unknown crystalline compounds. JCPDS-ICDD also will publish additional volumes in the NBS Crystal Data Determinative Table Series. The next two volumes, scheduled for 1983-1984, contain crystallographic data for more than 30,000 organic compounds collected by the NBS Crystal Data Center and the Cambridge Crystallographic Data Centre in the United Kingdom.

Diffraction data are used by scientists in industry, academia, and government research laboratories for characterization of solid crystalline structures and as an analysis for unknown materials. The JCPDS-ICDD/NBS agreement will ensure that reliable crystallographic data are available.

NBS/INTERAGENCY COOPERATIVE AGREEMENT FOR THE OPERATION OF THE CHEMICAL INFORMATION SYSTEM

The Chemical Information System (CIS) is an on-line service which provides access to a number of databases and computational programs of chemical interest. The CIS was initiated by the Environmental Protection Agency (EPA) and the National Institutes of Health. NBS and other federal agencies have subsequently joined in its development and operation. The system is used within these agencies, by their contractors and grantees, and by the general public. Interagency collaboration has led to efficiencies in operation of the CIS and helped users by providing a single focal point for a wide variety of chemical information. Funding for the system is provided by the cooperating agencies.

The signatory agencies to the cooperative agreement include, in addition to the three already designated, the Food and Drug Administration (FDA) and the Consumer Product Safety Commission (CPSC). Other agency participation includes the National Library of Medicine (NLM) and the National Cancer Institute (NCI).

In order to provide for the continued development and smooth operation of CIS the agencies have formed a Management Board. This Board, consisting of representatives of the cooperative agencies, establishes overall policy and goals, proposes an annual budget for submission to the individual funding agencies, establishes a schedule for database updates and system improvements, reviews and recommends addition of new components on the system, establishes procedures for assuring data quality, and provides general advice for the smooth operation and growth of the system.

In addition to participating in the CIS management function as the NBS representative, the Office of Standard Reference Data (OSRD) is contributing databases to the CIS system. These include the EPA/NIH Mass Spectral Data File, the NBS Tables of Thermodynamic Properties File and the Crystal Data Identification File. The proceeds from the sale of these databases are used by the OSRD to support CIS and other database activities.

PROGRAM STRUCTURE

Current activities in the Standard Reference Data program are carried out in 23 data centers and approximately 31 short-term projects located in the technical divisions of NBS and in academic and industrial laboratories. Each of these activities undertakes the collection and evaluation of the available data on a specified set of properties and substances. The activities are aggregated into three application-oriented program areas:

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

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

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

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

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

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

Publications in 1983

Series	Pages Published	Titles Published
JPCRD, Vol. 12	1087	25
NSRDS-NBS Series	21	1
Data Compilations from other publishers	176	1

Publications in 1983 (cont.)

Series	Pages Published	Titles Published
Other Publications in NBS Series	948	2
Bibliographies and indexes from other publishers	860	2
Machine-Readable Data Bases	-	2
Totals	3092	33

Subscribers to JPCRD

Month/Year	Number
9/1979	1237
9/1980	1234
9/1981	1265
9/1982	1234
9/1983	1230

Inquiries Received in OSRD

(Does not include inquiries received by data centers)

Year	Number
1979	882
1980	787
1981	657
1982	613
1983*	1210

Sales of JPCRD Offprints and Supplements

Year	Offprints	Supplements
1979	5981	137
1980	5079	111
1981	4254	137
1982	3567	266
1983*	3081	1666

*Projected to end of year

ENERGY AND ENVIRONMENTAL DATA

L. H. Gevantman, Program Manager

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

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

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

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

There is continued progress in the energy program, particularly relating to fusion energy. A publication on atomic energy levels of silicon has been issued. The work on atomic transition probabilities, particularly the transition metals, will be completed and published. Work of astronomic and atmospheric interest has been augmented with the issuance of two reports on the atomic energy levels of oxygen ions. Similarly laser technology and energy transfer phenomena have been addressed in three reports from the Atomic Collision Cross Section Data Center.

In the nuclear area, a report has been issued on atomic form factors and photon cross section data will soon appear on magnetic tape. The first volume of photonuclear data sheets covering hydrogen and helium has also been issued.

New directions in the Chemical Kinetics Data Center will address combustion and high temperature reaction processes. A manuscript covering the reactions of methane is almost complete. The high temperature kinetic rate constant data sheets project will continue with the publication of its first report in the Journal of Physical and Chemical Reference Data. New data sheets on the reactions of oxygen and hydrogen atoms with organic compounds will be issued in the coming year.

Environmental concerns have also been addressed in the program. Solubility data on coal derived substances have been evaluated and will be published in 1984. Data on oxygen and ozone solubilities have been published with nitrogen and air solubilities soon to follow. Similarly new efforts dealing with the distribution and ultimate fate data of chlorinated biphenyls in the environment have been undertaken.

In kinetics the new directions have import in tropospheric chemistry relating to smog formation and toxic substance production. Work on the kinetics of transients in solution continues with emphasis on photolytic as well as ionizing radiation processes. Two manuscripts will be completed in the coming year.

Close association with the IUPAC Solubility Data Project continues. A workshop on numerical data quality indicators was held at NBS under the joint sponsorship of the Chemical Manufacturers Association, the Environmental Protection Agency and the NBS. A report on the results has been issued. Similarly a symposium on Numerical Data Quality was held during the August-September ACS meeting and was well attended. The program's participation in the Chemical Information System (CIS) activities continue. The conversion of infra red data to digitized form has not yet taken place. It is anticipated that a contract will be let by the end of 1983. Other databases however, have been mounted on the CIS (Thermo and Xtal).

The data centers within the NBS as well as outside affiliates continue their progress to achieve automated data files for use within their respective centers. Some will also produce numerical data files on magnetic tape for use by the scientific public at large.

PUBLICATIONS IN 1983:

An Annotated Compilation and Appraisal of Electron Swarm Data in Electronegative Gases, J. W. Gallagher, E. C. Beaty, J. Dutton, and L. C. Pitchford, JPCRD, Vol. 12, No. 1.

The Solubility of Oxygen and Ozone in Liquids, R. Battino, T. R. Rettich, and Toshihiro Tominago, JPCRD, Vol. 12, No. 2.

Energy Levels of Silicon, Si I through SiXIV, W. C. Martin and R. Zalubas, JPCRD, Vol. 12, No. 2.

Small-Angle Rayleigh Scattering of Photons at High Energies: Tabulations of Relativistic HFS Modified Atomic Form Factors, D. Schaupp, M. Schumacher, F. Smend, P. Rullhusen, and J. H. Hubbell, JPCRD, Vol. 12, No. 3.

Chemical Kinetic Data Sheets for High-Temperature Chemical Reactions, N. Cohen and K. R. Westberg, JPCRD, Vol. 12, No. 3.

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Evaluated Theoretical Cross Section Data for Charge Exchange of Multiply Charged Ions with Atoms. I. Hydrogen Atom-Fully Stripped Ion Systems, J. W. Gallagher, B. H. Bransden, and R. K. Janev, JPCRD Vol. 12, No. 4.

Evaluated Theoretical Cross Section Data for Charge Exchange of Multiply Charged Ions with Atoms. II. Hydrogen Atom-Partially Stripped Systems, J. W. Gallagher, B. H. Bransden, and R. K. Janew, JPCRD, Vol. 12, No. 4.

Recommended Data on the Electron Impact Ionization of Light Atoms and Ions, K. L. Bell, H. B. Gilbody, J. G. Hughes, A. E. Kingston and F. J. Smith, JPCRD, Vol. 12, No. 4.

Selected Tables of Atomic Spectra; Atomic Energy Levels and Multiplet Table, O(IV), C. E. Moore, NSRDS-NBS 3 Section 10.

Selected Tables of Atomic Spectra; Atomic Energy Levels and Multiplet Tables, O(III), C. E. Moore, NSRDS-NBS 3, Section II.

Photonuclear Data - Abstract Sheets 1955-1982, Vol. 1 (Hydrogen-Helium) E. G. Fuller, H. Gerstenberg, NBSIR-83-2742.

Biweekly List of Papers on Radiation Chemistry and Photochemistry, A. B. Ross, Vol. 16.

Annual Cumulation of Papers on Radiation Chemistry and Photochemistry 1982, A. B. Ross, Vol. 15.

INDUSTRIAL PROCESS DATA

H. J. White, Jr. Program Manager

The chemical industry has continuing need for reference data. The design of every piece of equipment involves a calculation requiring input and output specifications and data on the properties of the substance or substances concerned. The types of data most frequently needed are data on thermodynamic and transport properties. This program is designed to provide these data.

Interest in reference data has increased in the chemical industry in recent years. Evidence for this is given by the rapid development of DIPPR, the industry's own reference data program, which is carried out under the auspices of the American Institute of Chemical Engineers. There are several reasons for this increased interest. The increasing use of the computer in the design process is one. The speed and flexibility of the computer allow the design engineer to evaluate many options and to optimize the design according to various strategies. Another is the desire to minimize overdesign so as to improve productivity and lower the break-even point for utilization of the process. There will always be uncertainties in data and calculations for which the design engineer compensates by overdesigning. However, if good design data are available, the design engineer can work to closer tolerances and minimize overdesign.

For administrative purposes, it is convenient to group thermodynamic activities. Those which involve chemical reactions and which can be called thermochemical processes form one group, and those in which the substances involved retain their identities throughout the process and which can be called thermophysical form another. The expansion of steam through a turbine is an industrially important example of the latter. In addition, thermodynamic processes can be grouped in accordance with whether they involve single substances or mixtures or solutions. Both categories are important. Industry necessarily deals extensively with mixtures, however, the understanding of the behavior of single substances is also industrially important and provides the basis for treatments of mixtures. Thermochemical or thermophysical processes can, of course, involve either mixtures or single substances. The program in industrial process data is balanced to provide attention to thermochemical and thermophysical processes, single substances and mixtures. Transport properties are grouped with the thermophysical processes. The program for each data center or project is described separately.

There are two major thrusts that currently influence the activities in most data centers and many projects. These are automation and cooperative activities. They are not unrelated because often the key to effective cooperative activities involves the easy exchange of databases and other products between data centers and the checking of the evaluations of one group by another. A level of automation which supports such easy exchanges thus assists cooperative activities.

The program on industrial process data is cooperating with DIPPR, which has been mentioned already, in a variety of ways. One is the development of automated versions of DIPPR's reference data compilation. Other cooperative activities involve the development of internationally recognized steam tables in cooperation with the International Association for the Properties of Steam,

and internationally agreed upon tables of chemical thermodynamic data under the auspices of CODATA. The latter activity has required extensive development of specialized software.

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Thermodynamic Properties of Steam in the Critical Region, J. M. H. Levelt Sengers, B. Kamgar-Parsi, F. W. Balfour, and J. V. Sengers, JPCRD Vol. 12, No. 1.

Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. VII. Other Carbon Backbone Polymers Umesh Gaur, Brent B. Wunderlich, and Bernhard Wunderlich, JPCRD Vol. 12, No. 1.

Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. VIII. Polyesters and Polyamides, Umesh Gaur, Suk-fai Lau, Brent B. Wunderlich, and Bernhard Wunderlich, JPCRD Vol. 12, No. 1.

Evaluation of Binary PTxy Vapor-Liquid Equilibrium Data for C_6 Hydrocarbons. Benzene + Hexane, Buford D. Smith, Ol Muthu, and Ashok Dewan, JPCRD Vol. 12, No. 2.

Evaluation of Binary Excess Enthalpy Data for C_6 Hydrocarbons. Benzene + Hexane, Buford D. Smith, Ol Muthu, and Ashok Dewan, JPCRD Vol. 12, No. 2.

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Thermodynamic Properties of D_2O in the Critical Region, B. Kamgar-Parsi, J. M. H. Levelt Sengers and J. V. Sengers, JPCRD Vol. 12, No. 3.

International Tables of the Surface of Water, N. B. Vargaftik, B. N. Volkov and L. D. Voljak, JPCRD Vol. 12, No. 3.

A Correlation of the Viscosity and Thermal Conductivity Data of Gaseous and Liquid Ethylene, P. M. Holland, B. E. Eaton and H. J. M. Hanley, JPCRD Vol. 12, No. 4.

Transport Properties of Liquid and Gaseous D_2O over a Wide Range of Temperature and Pressure, N. Matsunaga and A. Nagashima, JPCRD Vol. 12, No. 4.

Thermochemical Data for Gaseous Monoxides, J. B. Pedley and E. M. Marshall, JPCRD Vol. 12, No. 4.

Vapor Pressures of Coal Chemicals, J. Chao, C. T. Lin, and T. H. Chung, JPCRD Vol. 12, No. 4.

Manual for Predicting Chemical Process Design Data Data Prediction Manual, R. P. Danner, and T. E. Daubert, Design Institute for Physical Property Data, American Institute of Chemical Engineers.

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

Thermophysical Properties of Helium, Magnetic Tape 5, Magnetic data tape available from the Office of Standard Reference Data.

Interactive Fortran Program to Calculate Thermophysical Properties of Six Fluids, Magnetic Tape 6, Magnetic data tape available from the Office of Standard Reference Data.

MATERIALS PROPERTIES DATA

J. R. Rumble, Jr., Program Manager

The past year has been an exciting one for the Materials Properties Data Program. Highlights include major compilations of evaluated data, cooperative agreements on joint data activities with technical societies, and new data evaluation activities. The program has five components as shows in Table 1. In each area, projects are underway and new activities are planned, depending on funding.

The work is accomplished in a variety of ways. Four ongoing data centers exist: Crystal Data, Alloy Phase Diagrams, Phase Diagrams for Ceramists, and Corrosion. The latter is new as of 1983. Each of these has cooperative agreements linking its activities to major outside technical groups (Table 2). This ensures that the data center work addresses the needs of the U.S. research and technical communities. Projects are often jointly funded and, in some cases, substantial amounts of industrial support have been raised for these programs.

OSRD also sponsors a number of short-term evaluation projects that address specific data needs within the framework given in Table 3. These are handled both inside and outside NBS. Often these represent pilot projects within new programs to demonstrate feasibility and types of output, to serve as models for larger efforts, and to get the programs going.

Finally, a major part of the program is to help user groups articulate their evaluated data needs, set up structures to address them, and find necessary support. In the past year several such efforts have taken major steps forward, especially in the area of mechanical properties data.

Let us touch on the highlights within each component, new areas of activity will also be pointed out.

Structure and Characterization

The structure and characterization of solid materials is extremely important. The identification of unknown substances has always been a major use of evaluated data. The NBS Crystal Data Center has developed powerful techniques for rapidly identifying crystalline substances. Computer-readable databases supporting this work are being distributed, and it is hoped that they will be integrated into diffractometers within the next few years. The NBS Crystal Data Center this year published Volumes V and VI of the Crystal Data Determinative Tables Series. These volumes contain data on over 25,000 compounds as collected by the Cambridge Crystallographic Data Centre. The NBS Data Center interaction with the International Centre for Diffraction Data-JCPDS (ICDD-JCPDS) continued on a high note. Next year, the ICDD-JCPDS will have a research associate at the NBS center working on software to be used with the NBS Crystal Data Identification File.

Surfaces as well as bulk materials have received a great deal of attention, especially with progress in miniaturization of electronic components and catalysis. Over the last 20 years, a number of techniques involving electron and photon spectroscopies have been developed to characterize surfaces, and

the data generated is in need of evaluation. One project on ESCA data is underway, but many more are needed. During the next year, OSRD will be working with the Surface Science Division in the Center for Chemical Physics to develop priorities and begin addressing them.

Physical Properties

In this area, needs for evaluated data on superconducting materials have been presented to OSRD. Depending on funding, a project will be established in this area. Funding for the Diffusion in Metals Data Center was eliminated, beginning FY 84. This center has completed a definitive volume of evaluated diffusion data for copper and its alloys. As new needs for diffusion data become apparent, projects will be established.

Phase Equilibria

NBS, through the Center for Materials Science (CMS) and OSRD, has three major programs for evaluating phase data for alloys, ceramics, and polymeric blends. These major programs are well-integrated into the user communities, and significant progress was achieved in all three this year.

The Alloy Phase Diagram Center is the focal point of the NBS/American Society of Metals (ASM) joint program to evaluate all alloy phase diagrams. Over the last year, the Alloy Center has continued to exert vigorous technical leadership. A major data evaluations workshop was held, the Bulletin of Alloy Phase Diagrams published over 50 new diagrams, and work on prototype databases began seriously. OSRD supports the program in two major ways: direct support of the data center and support of individual evaluation projects (see Table 3).

The Phase Diagrams for Ceramists Data Center concluded a major agreement with the American Ceramics Society (ACerS) which strengthens their joint program on evaluated data. ACerS has begun fund-raising efforts, and the NBS data center has established vigorous programs in database graphics and thermodynamic modeling. In addition, new systems such as molten salts are receiving attention.

Phase data for polymeric blends are important in developing new and improved polymers. NBS and the Society of Plastics Engineers (SPE) have concluded an agreement for a joint program to generate reference data in this area. The program will build on the existing data group at NBS and this year will identify an appropriate pilot project.

Performance Properties

Corrosion

The economic impact of corrosion in the U.S. was estimated to be about $125 billion in 1982. Clearly this effort could be substantially reduced by application of more resistant materials. The National Association of Corrosion Engineers and NBS signed a cooperative agreement last year which will provide the technical community with evaluated corrosion data. The Metallurgy Division (CMS) and OSRD have established the NBS Corrosion Data Center to act as the technical focal point of this program. This year an

initial pilot project has been started to define criteria for evaluation of corrosion rate data and apply them to data for stainless steel in chloride solutions. Other projects will be started in 1984 in the area of stability diagrams for Fe systems with emphasis on their computer generation.

Mechanical Properties

OSRD has been working closely with outside groups to address a variety of problems related to mechanical properties data. In particular, the Metals Properties Council (MPC) has developed a major effort to provide computerized access to materials property data. The Office has interacted strongly with this project and has developed a four-pronged effort involving data evaluation, data standardization, database creation, and user workshops.

The evaluation of mechanical properties data until now has been concentrated in areas of high technology such as nuclear power generation and aerospace. Working with other groups, such as ASME and MPC, OSRD is interested in seeing established a broader scope of activity that will positively affect the quality of data in less esoteric applications. Several projects are being planned for the next year.

Computer access to mechanical properties data will cause new problems with respect to standardization of data generation and reporting. Data on computers can quickly lose its pedigree, be combined incorrectly with inappropriate data, and misused in other ways. OSRD has had conversations with ASTM and SAE about rethinking present standards and looks forward to progress in this area. To provide a basis for understanding, OSRD has started a project with General Electric to examine the problems associated with a small set of properties and materials.

The MPC materials property data network will involve linking together many databases on a variety of properties created by interested parties. For such a system to be useful, more databases must be created from the new existing published compilations. MPC and OSRD will work together to persuade publishers, societies, and other groups to begin building the needed databases more intensely.

Last November OSRD, in conjunction with CODATA and Fachinformationszentrum (West Germany), sponsored a Workshop on Computerized Materials Data Systems. This workshop was attended by 75 persons who recommended that the interested groups, industry, technical societies, and Government begin immediately to bring such capability into being. The MPC has recognized this strong endorsement of their effort and is moving ahead.

A key ingredient to success in this type of project is strong user input from the beginning. To this end, NBS and MPC have set up a series of user workshops to be held next year addressing the needs in each of three application areas: ground transportation, nuclear power generation, and aerospace. These workshops will be sponsored by groups including NBS, MPC, EPRI, SAE, ASM, and AIAA. From the the workshops will hopefully come detailed needs and the way will be paved for industrial acceptance and support of the system.

Summary

Inherent in all the above activity is the need for increased resources. At present, OSRD has stretched its existing resources extremely thin. The industrial community has turned to OSRD for leadership, and OSRD is working to provide. A major effort this year will be mounted to attract from NBS and other government agencies the attention these activities deserve and to turn that attention into direct support.

Table 1

OSRD Materials Properties Data Program

- Structure and Characterization
- Physical Properties
- Phase Equilibria
- Performance Properties
  - Corrosion
  - Mechanical Properties

Table 2

Major NBS-Outside Data Agreements

American Society of Metals	(Alloy Phase Diagrams)
American Ceramic Society	(Phase Diagrams for Ceramists)
Internal Centre for Diffraction Data-JCPDS	(Crystal Data)
Society of Plastics Engineers	(Polymeric Blend Phase Diagrams)
National Association of Corrosion Engineers	(Corrosion Data)

Table 3

OSRD Material Properties Data Program

Structure and Characterization

- Crystallography
  - NBS Crystal Data Center
  - JCPDS - ICDD
  - Cambridge Crystallographic Data Centre
  - Cation-Nitrogen Distance (U. Ill.-Chicago)
- Surfaces
  - ESCA data Project - Surfax, (CA)

Physical Properties

- Optical
  - Refractive Index - CINDAS (Purdue)
- Superconductivity (not yet funded)

Phase Equilibria

- Alloys
  - NBS Alloy Phase Diagram Data Center
  - NBS/ASM Phase Diagram Program
    - Fe, Al, Ti - NBS
    - V, Nb - Ames
    - Cr - U. Alabama
    - Cu - Carnegie-Mellon
    - Rare Earths - Iowa State
    - Alkalis - Montreal
- Ceramics
  - NBS Phase Diagrams for Ceramists Data Center
  - Molten Salts - Montreal
- Thermochemistry
  - Thermochemistry of Alloy and Elements - CINDAS (Purdue)

Corrosion

- NBS Corrosion Data Center
- NBS/NACE Corrosion Data Program
  - Stainless Steels in Aqueous Chlorides - Georgia Tech

Mechanical Properties

- Computerized Materials Data Systems
  - Metals Properties Council
  - Data Standardization - General Electric
  - Data Validation - (not yet funded)

PUBLICATIONS IN 1983:

Diffusion Rate Data and Mass Transport Phenomena for Copper Systems, Part II, D. B. Butrymowicz, Volume 8 of the INCRA Series on the Metallurgy of Copper (International Copper Research Association, Inc., New York), 701 pp.

"Crystal Data Determinative Tables." U. S. Department of Commerce, National Bureau of Standards and the JCPDS--International Centre for Diffraction Data, Swarthmore, PA, Vol. 5, 3rd edition (in press).

"Crystal Data Determinative Tables." U. S. Department of Commerce, National Bureau of Standards and the JCPDS--International Centre for Diffraction Data, Swarthmore, PA, Vol. 6, 3rd edition (in press).

Space-Group Frequencies for Organic Compounds, A. D. Mighell, V. L. Himes and J. R. Rodgers, Acta Cryst., A39, (in press).

Bulletin of Alloy Phase Diagrams, Vol. 4 (1983).

Includes NBS evaluations for:

Ti-Cu	Fe-Ru	Al-Na
Al-Be	Ti-Au	Al-Sn
Al-Zn	Al-In	
Ti-Ag	Ti-Cd	
Al-Ga	Fe-Os	

AUTOMATION

J. R. Rumble, Jr., Program Manager

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

The highlights of this year's activity include releasing two new databases, the arrival of a new NBS typography system and the installation of a dedicated data center facility.

Numerical Databases

Two new NBS Standard Reference Databases have been released to the public. They are "Thermophysical Properties of Helium" and the "Interactive Fortran Program to Calculate Thermophysical Properties of Six Fluids" (NBS Standard Reference Databases 5 and 6). Both are interactive programs which calculate reference data from well-treated models.

OSRD now has six databases available (Table I). In addition, three of them are available on various on-line networks.

Table I

NBS STANDARD REFERENCE DATABASE	On-line Availability
1. NBS/NIH/EPA/MSDC Mass Spectral Data Base	CIS, Questel
2. NBS Chemical Thermodynamics Data Base (NBS Tech Note 270)	CIS
3. NBS Crystal Data Identification File	CIS, CISTI
4. NBS Thermophysical Properties of Hydrocarbon Mixtures (TRAPP)	
5. Thermophysical Properties of Helium	
6. Interactive Fortran Program to Calculate Thermophysical Properties of Six Fluids	

Activities in this area for the coming year include creation of a database for the JANAF tables and the writing of software packages for The Chemical Thermodynamics, Single Crystal ID File and JANAF databases. These packages could be distributed with the database. Also, if time permits, the three interactive programs will be adapted to BASIC and put on a media suitable for personal computers.

Computing Facilities

Two substantial improvements to OSRD computer hardware and software were made in 1983. First, a standard typography system was obtained by NBS which will replace the GPSDC system previously used. The vendor supported product made by Bedford will greatly increase OSRD's ability to produce the complicated manuscripts common among our publications.

In addition, OSRD's HP1000 computer and associated software is now operational and being used. We have configured it identically to the other HP1000 in The Center for Chemical Physics and anticipate extensive usage and cooperation for data entry and database work.

Database Activities

The emphasis of OSRD's internal effort over the past year has been in setting in place the tools described above. OSRD also sponsored for the data centers a course in Modern Programming Practices in which the concepts of structural programming and design were presented. This week-long course was very well received.

Individual data centers continued to make great progress in their database efforts. Table II summarizes the on-going projects in this area.

Table II

OSRD Activities in Numerical Data Bases

Crystal Data

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

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

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

Atomic Spectra
- Energy Levels
- Transition Probabilities

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

Properties of Fluid Mixtures
  Hydrocarbons
  Polar Molecules
  Helium

Collision Cross-Sections
  Electrons
  Photons and Charged Particles

Other Activities

OSRD has become a resource for outside groups who want to build numeric databases in science. Over the past year, a large number of groups have been in contact with various staff members. These efforts, which include working with The Metals Properties Council, AIChE DIPPR project, Chemical Information System (NIH, EPA), ASM and IUPAC, have been very fruitful.

DATA CENTER AND PROJECT REPORTS

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

ALLOY PHASE DIAGRAM DATA CENTER

Kirit Bhansali, Director
Center for Materials Science, NBS

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

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

A vigorous evaluation program for titanium systems, with support by ONR, is now well in its fourth year, and more than 25 titanium binary systems have been evaluated. Evaluation of aluminum systems has begun, and ten aluminum binary systems have been completed. This work is supported in part by DARPA. In addition, work on iron systems has started. During this evaluation effort, thermodynamic optimization programs have been enhanced and interfaced with the graphics software.

Work for designing and creating a database of phase information and ancillary data is underway. This is being done in close cooperation with the ASM.

AQUEOUS ELECTROLYTE DATA CENTER

David Garvin, Director
Center for Chemical Physics, NBS

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

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

A database of activity and osmotic coefficients and excess Gibbs energies has been compiled for approximately 400 aqueous binary electrolyte solutions. The base contains coefficients for fitting equations for each electrolyte solution which can be used to calculate activity and osmotic coefficients at a selected molality. An extended Pitzer equation has been applied to 110 electrolyte solutions. All of these activities apply to 25 °C.

Procedures have been developed to calculate the excess, apparent molar and partial molar properties of aqueous solutions which associate, hydrolyze

or hydrate. Excess Gibbs energy, excess enthalpy and heat capacities can be calculated. These procedures are expected to provide a necessary base for extending the interpolative and predictive capabilities of the Center to higher temperatures, mixtures, and complexing ions.

A paper discussing the solubility of gypsum and of chromium ion and its complexes and a series of bibliographies on aqueous solutions of CO_2, H_2S, H_2SO_4, NH_3 and $CuCl_2$ have been prepared for DIPPR.

ATOMIC COLLISION CROSS SECTION DATA CENTER

Jean W. Gallagher, Director
Center for Basic Standards, NBS

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

In the past year the Center has collaborated with a number of visiting scientists and JILA staff members to produce evaluated data publications. Three will appear in this year's issues of the Journal of Physical and Chemical Reference Data (JPCRD). Two additional manuscripts are being finalized for publication next year.

In addition, two new projects were initiated. The first concerns data on the charge transfer of hydrogen and deuterium atoms, and molecules and their ions with metal vapors; the second concerns an update of the Multiphoton Cross Section bibliography. Other new projects will be initiated in 1984. Continued effort will be directed toward the automation of the data center files.

ATOMIC ENERGY LEVELS DATA CENTER

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

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

Energy levels for Si(I-XIV), and O(III) and O(IV) were published in the Journal of Physical and Chemical Reference Data. More than half of the updating of the isoelectronic sequences in the iron group series was completed. Other contributions were made to the literature in atomic spectroscopy such as a report to the NAS-NRC Line Spectra Committee on "Systematics and Regularities in Atomic Spectra."

Future efforts will involve completion of the energy level compilation of the iron group elements. Work on the energy levels of P(I-XV) will also continue. A bibliography on atomic energy levels (Supplement III) will be issued covering the period July 1979 to December 1983. Automation of the data file and close collaboration with the Atomic Transition Probabilities Data Center will continue.

ATOMIC TRANSITION PROBABILITIES DATA CENTER

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

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

The atomic transition probability data tables for the allowed lines of the elements scandium through nickel will be completed this year. Work is now in progress to compile and evaluate the forbidden lines of these elements. Effort to create an automated data file continue in cooperation with the Atomic Energy Levels Data Center and with the OSRD.

Future plans call for the completion of the work on scandium through nickel. Efforts will be initiated on the transition probabilities of hydrogen through neon with emphasis on C, N_2, O_2 and Ne. Work on selected heavy elements (Kr, Zr) will also be started. Continued effort will be invested in data file automation with the goal of an operative system at the end of calendar 1984.

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

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

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

Work on a series of publications on the viscosity, thermal conductivity and heat capacity of a set of seventy-six fluids of industrial importance is nearing completion. Other OSRD projects involve evaluated optical property data and thermochemical data for alloys and elements.

CHEMICAL KINETICS DATA CENTER

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

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

Approximately, 250 data sheets on elementary reactions relating to pyrolysis and oxidation of simple hydrocarbons are nearly complete. A manuscript on the elementary combustion reactions of methane will be submitted for publication. Kinetic data for atmospheric reactions of halogen-containing species were evaluated. A manuscript on this subject will be completed this year.

Some shift in emphasis will take place during the next year due to the maturation of the data on stratospheric reactions and an increase in demand for data on combustion kinetics. Preparation of evaluated kinetic rate constants for high temperature combustion reactions will be initiated. The manuscript on methane combustion will be finalized and submitted for publication. Effort toward automating the kinetic data file will continue.

CHEMICAL THERMODYNAMICS DATA CENTER

David Garvin, Director
Center for Chemical Physics, NBS

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

With the publication of "The NBS Tables of Chemical Thermodynamic Properties" the Center has cleared the way for further development of its techniques. A major purpose is full automation of the Center's activities. This will promote internal efficiency and flexibility and pave the way for easier, more effective cooperation with other data projects. A standardized procedure has been established for entry of bibliographic data into the system and preliminary versions exist for reaction catalogs and for the extraction of data from experimental papers.

The Center is cooperating with four others to produce a set of prototype tables for CODATA. These tables covering a number of compounds of calcium and some auxiliary substances will serve two purposes. One, they will demonstrate the feasibility of producing chemical thermodynamic tables through the cooperative activities of a number of data centers in accordance with the system outlined in CODATA Bulletin No. 47, "A Systematic Approach to the Preparation of Thermodynamic Tables." Two, they will provide a model for a new generation of tables and make them available for review and comment within the thermodynamic community. It should also be mentioned that preparation of the tables has provided practical experience to those involved in the preparation of tables using a decentralized highly-automated system.

The Center has prepared the Inorganic Section of the Bulletin of Chemical Thermodynamics as well as the index to the entire Bulletin. The Bulletin is published annually.

CORROSION DATA CENTER

G. M. Ugiansky, Director
Center for Materials Science, NBS

The Corrosion Data Center was established in 1983 to provide evaluated corrosion data to the technical community. It provides technical coordination for the NBS-NACE Corrosion Data Program.

The Center has begun with two pilot projects. The first is concerned with developing evaluation criteria for corrosion rate data and applying them to corrosion of stainless steel in chloride solutions. The second involves computer generation of chemical stability diagrams (also known as Pourbaix diagrams) and how to integrate kinetics into them.

CRYSTAL DATA CENTER

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

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

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

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

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

DIFFUSION IN METALS DATA CENTER

John Manning, Director
Center for Materials Science, NBS

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

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

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

FLUID MIXTURES DATA CENTER

Neil Olien, Director
Center for Chemical Engineering, NBS

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

A second volume to "Thermophysical Properties of Fluids" has been prepared. "Thermophysical Properties of Fluids II" covers the C_1 - C_4 aliphatic hydrocarbons. As with the first volume the same set of equations is used for the thermodynamic and transport properties of all of the fluids so that change from one fluid to another simply involves substitution of a different set of coefficients. This provides a considerable simplification in the computer generation of data for these substances. The two volumes combined will cover 11 fluids.

Thermophysical Properties of Fluids I, TRAPP, and a set of thermodynamic properties for helium are now available in tape form.

New formulations for the thermodynamic properties of CO and H_2S have been prepared, the latter with funding from GRI. A custody-transfer equation for CO_2 is being prepared as is an equation of state for CO_2 in the supercritical region, both with industrial support.

Technical problems involving prediction of the saturated surface have slowed the development of formulations for the CH_4/C_2H_6 and CH_4/N_2 mixtures.

FUNDAMENTAL CONSTANTS DATA CENTER

Barry N. Taylor, Director
Center for Basic Standards, NBS

The Center provides a centralized source of information on the fundamental physical constants and on closely related precision measurements. The Center

participates in the periodic development of sets of "best" or recommended values of the fundamental physical constants by means of least-squares adjustments. The self-consistent best values of the constants resulting from an adjustment are required for computational purposes and often are the basis for other data compilations.

A volume was published on the analysis of fundamental constants entitled, "Numerical Comparisons of Several Algorithms for Treating Inconsistent Data in a Least-Squares Adjustment of the Fundamental Constants" (NBSIR 81-2426). The 1983 Least-Squares Adjustment of the Fundamental Constants will be published in 1984.

ION ENERGETICS DATA CENTER

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

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

The evaluation on the heats of formation of gaseous ions and related data continues. Approximately 2000 species have been covered. This effort has the cooperation of three additional experts from outside the data center. A comprehensive compilation and evaluation of gas phase proton affinities has been completed. A manuscript is in process of being written.

Future activity will concentrate on the completion of the evaluation on ion heats of formation and the submission of a manuscript on proton affinities for publication. Some attention is also being given to compiling rate constants for ion-molecule reactions. Finally, continued emphasis will be given to the automation of data center files and activities.

JANAF THERMOCHEMICAL TABLES

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

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

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

The JANAF Center is one of the five centers involved in the preparation on the prototype CODATA tables.

MOLECULAR SPECTRA DATA CENTER

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

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

A manuscript on microwave spectra of SO_2 has been submitted and is presently being reviewed. A magnetic tape containing the "Spectral Line Atlas of Interstellar Molecules (SLAIM) has been produced. Documentation of the tape is almost complete. The Atlas contains the spectral characteristics for all 55 known interstellar species. Finally, the evaluation of data for "Microwave Spectral Tables of Hydrogen Species" has been partially completed.

In the coming year the SO_2 paper will be published and the evaluation of microwave spectra of hydrocarbons will be completed. An infrared calibration atlas to cover the frequency range 500 to 720 cm^{-1} will be prepared using spectra of OCS, N_2O and CO_2.

MOLTEN SALTS DATA CENTER

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

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

Selected properties on single and multicomponent molten salt systems have been published in the Journal of Physical and Chemical Reference Data. A summary publication combining and updating all salt systems evaluated to date is in its preliminary stages of preparation. Considerable progress has been achieved in automating the bibliographic file at the data center. It is now accessible on the main computer at R.P.I. Additionally a magnetic tape on molten salt eutectic mixture data is in its final stages of preparation.

Future efforts will be directed toward completion of the comprehensive volume on molten salt properties. Some preliminary effort will be given over to compiling and evaluating various physical properties of highly concentrated salt solutions. Automation of the data will continue.

NATIONAL CENTER FOR THE THERMODYNAMIC DATA OF MINERALS

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

The Center compiles, indexes, and evaluates data on the thermodynamic and thermophysical properties of minerals, their synthetic analogs, and geologic materials. These data are important for geochemical purposes and useful

industrially in the fields of metallurgy and the synthesis and production of inorganic chemicals.

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

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

PHASE DIAGRAMS FOR CERAMISTS DATA CENTER

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

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

The PDFC Center has published jointly with the American Ceramic Society the series " Phase Diagrams for Ceramists." Volume 5 contains 650 diagrams of molten salts, sulfides, and oxynitride systems; work on this volume was completed and published this year. Evaluation work for Volumes 6 and 7 has started.

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

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

PHOTON AND CHARGED PARTICLE DATA CENTER

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

The Center compiles, evaluates, and disseminates data on the interaction of ionizing radiation with matter. The data on photons and charged particles

include single-scattering cross sections and transport data pertaining to penetration of radiation through bulk matter.

A report on atomic form factors used in determining photon scattering cross sections has been published in the Journal of Physical and Chemical Reference Data. In addition, an evaluated photon cross section data file has been prepared on magnetic tape. The data cover the energy region from 1 keV to 100 GeV and all elements from Z=1 to 100. The data include cross sections for scattering, photoelectric absorption, and pair production as well as attenuation coefficients. The tape is being documented and will be available next year. The first volume (hydrogen and helium) in a series of photonuclear reaction data reports has been issued as an NBS internal report.

Future effort will involve the completion and delivery to OSRD of the magnetic tape, and the initiation of data projects dealing with heavy particle stopping power and bremsstrahlung cross sections data covering energies up to 1000 MeV.

RADIATION CHEMISTRY DATA CENTER

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

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

A compilation on triplet-triplet absorption spectra for approximately 600 organic molecules is nearing completion. Triplet yield data are being compiled and evaluated for future publication. Another project which compiles one-electron reduction potentials of radical species in aqueous solution has been initiated. Rate constants for O_2 and HO_2 reactions in aqueous solution are being updated with a view toward a future publication. The Biweekly list of Papers on Radiation Chemistry and the Cumulative Index, Vol. 16 and Vol. 15 respectively were also published.

In addition, progress on the build-up of an automated numeric data file is being made. The data will be indexed by CAS registry numbers, molecular formula and chemical name. Approximately, 14,000 chemical species are entered in the file. An automated bibliographic file (RCDC bib) is now mounted on the DOE RECON system which is run by the Technical Information Center in Oak Ridge, Tennessee.

Future efforts will be devoted to the publication of the evaluative efforts mentioned above and the assembly on magnetic tape of approximately 6000 reaction rate constants of transient species in aqueous solution. The successive volumes of the Biweekly Lists and the Cumulative Index will also be published.

THERMODYNAMIC RESEARCH CENTER

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

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

The Center has continued its work on the thermodynamic properties of organic substances containing the atoms C, H and O in the C_1 - C_4 range. A substantial number of major industrial products and intermediates is included in this group. Entropies and enthalpies for the condensed phases of all substances in the group for which low-temperature heat-capacity data are available have been gathered and evaluated. A paper is in the publication process. In another part of the same project, ideal-gas thermal functions have been prepared for those molecules in the group for which sufficient data are available. A report is in the review process. Finally, reactions involving compounds in the group for which calorimetric or equilibrium data are available are being studied. The intent of the project is to utilize these resources to obtain a network of thermodynamically consistent data for as many compounds in this group as possible.

Data on organic substances are being systematically entered into the CIS systems. The data serve to test the software of the thermo module of the CIS system which the Center was instrumental in preparing. They also serve to establish a useable base of data on organic compounds on the CIS system.

The Center has prepared the current section on organic compounds in the Bulletin of Chemical Thermodynamics. The Bulletin is published annually.

THERMODYNAMIC RESEARCH LABORATORY

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

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

A comprehensive review has been made of the C_6 - C_6 systems. The available data on excess volume, excess enthalpy, PTxy measurements and PTx measurements have been compiled and evaluated. Papers on the benzene-hexane and benzene-cyclohexane systems have been published and papers on other systems are being prepared. Work is also being done on C_6 and C_7 systems and systems involving an aliphatic alcohol and a hydrocarbon.

The evaluation process has been highly automated and eventually evaluated data will be made available in automated form.

CRITICAL COMPILATION OF MASS SPECTRAL DATA

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

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

CRITICAL EVALUATION OF HIGH TEMPERATURE KINETIC DATA

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

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

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

WATER SOLUBILITY AND RELATED PARAMETERS OF COAL DERIVED COMPOUNDS

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

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

A manuscript has been submitted and reviewed. The paper will be published in the Journal of Physical and Chemical Reference Data in 1984.

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

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

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

The publication on O_2 and Ozone was published in the Journal of Physical and Chemical Reference Data. A manuscript for nitrogen and air in liquids has been reviewed and will be published in 1984.

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

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

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

To date, a draft on the solubility of mercury salts is in final stages of completion. The data on the other salts, zinc and cadmium are presently being evaluated. The mercury manuscript will be published in 1984.

COMPILATION OF SPECTROSCOPIC DATA BELOW 2000 ANGSTROMS

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

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

The manuscript and data tables have been submitted on magnetic tape. Some difficulty has been encountered in producing a final manuscript. However, these should be overcome in the near future and a manuscript delivered in early 1984.

K SHELL IONIZATION BY HYDROGEN AND HELIUM IONS

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

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

The data have now been collected through July 1983. Two programs have been written to order the data to a scaled projectile velocity variable to permit statistical analysis. Completion of the project is now estimated by September 1984.

CRITICAL EVALUATION OF CHEMICAL KINETIC DATA FOR METASTABLE ELECTRONICALLY EXCITED SPECIES

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

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

Progress continues. A manuscript will be delivered in December 1983.

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

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

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

This project has been completed.

A final manuscript is being assembled and will be delivered by the end of 1983. Data for all of the lithium systems and a few sodium and calcium systems will be included.

A CRITICAL REVIEW OF POLYCHLORINATED BIPHENYL PHYSICAL - CHEMICAL DATA OF ENVIRONMENTAL RELEVANCE

D. Mackay
University of Toronto
Ontario, Canada
Source of Support: DOE

A critical review of the relevant thermodynamic and transport properties of polychlorinated biphenyls will be done. Nine properties will be assessed and an attempt to correlate these properties with "chlorine number" will be made. These relationships will be used to predict property values for those substances where no experimental values exist. Data for approximately 50 related compounds will be produced and procedures will be established for further applications. A report will be submitted for publication in 1984.

DATA ON AQUEOUS ELECTROLYTES

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

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

This project and a previous one have been concerned with methods for the evaluation and representation of data over a range of temperatures and pressures. This problem necessarily involves the inclusion of internal equilibria in solutions.

Further studies will be made of techniques for computer transfer of data files between Delaware and the Aqueous Electrolyte Data Center at NBS.

DIPPR DATA PROJECTS

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

DIPPR supports a number of data compilation, evaluation, and prediction projects with cooperative funding from industry and Government. In accordance with an agreement between NBS and AIChE, the parent organization of DIPPR, DIPPR and NBS will cooperate in a variety of ways in the production of critically evaluated data for industry.

At the present time, NBS is supporting 3 DIPPR activities: the preparation of a data prediction manual, preparation of a data book on phase equilibria in aqueous electrolyte systems, and development of software to provide interactive computer access to the DIPPR data compilation. The first 5 chapters of the data prediction manual have been published recently and work is continuing on other chapters. The data compilation has been completed for the first 200 odd substances and is in the process of publication. Since the compilation is expected to contain more than 1000 substances in time, there is interest in the preparation of an interactive automated database as an alternative output. NBS is supporting the development of this automated database. The data book on aqueous electrolyte systems will contain necessary computational techniques, examples illustrating their use in industrial calculations, and standard reference and annotated reference lists for additional data.

EQUILIBRIUM AND TRANSPORT PROPERTIES OF POLYATOMIC GASES AND THEIR MIXTURES AT LOW DENSITY

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

The investigators have devised techniques to determine the intermolecular potentials for simple molecules from thermodynamic data. In a previous project, these techniques were used to derive definitive data for the thermodynamic and transport properties of the noble gases and their mixtures at low densities. The results of this work are in press.

Attempts will now be made to apply these techniques to a somewhat more complex set of fluids: H_2, N_2, O_2, CO, CO_2, N_2O and CH_4. The intent is to provide definitive data on the equilibrium and transport properties of these gases and their mixtures in the region of low density.

PREPARATION OF POURBAIX DIAGRAMS FOR SELECTED SYSTEMS

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

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

Final reports are in preparation on the systems Fe-O-H and Fe-H_2O. The systems O-C, C-Fe and O-H-C are under investigation and work is starting on the system O-H-C-Fe.

PROPERTIES OF POLAR FLUIDS

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

A formulation for the density and thermodynamic properties of water prepared under this project had been endorsed by the International Association for the Properties of Steam as the "Provisional IAPS Formulation 1982 for the Thermodynamic Properties of Ordinary Water Substance for Scientific and General Use." The formulation has been carefully tested by national committees in 8 countries. An IAPS Release on the formulation is in preparation and "steam tables" incorporating the formulation have been written and are in press. Releases on transport properties incorporating the new release have also been prepared.

The formulation will not be investigated as a basis for the treatment of mixtures.

THERMOPHYSICAL PROPERTIES DATA FOR FLUIDS

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

This project is concerned with the development of comprehensive formulations for the thermodynamic and transport properties of fluids. This includes formulations providing an accurate description of the behavior in the critical regions.

A comprehensive survey has been made of the properties of water in the critical region (because of waters' importance the data are unparalleled in quantity and quality). Comprehensive formulations for the thermodynamic and transport properties for both ordinary and heavy water in the critical region have been prepared and are being published. In addition, formulations for the transport properties of ordinary and heavy water have been prepared for the International Association for the Properties of Steam based on the recently endorsed thermodynamic formulations for these substances (see elsewhere in this report).

The techniques for preparing formulations for the thermodynamic and transport properties in the critical region which have been developed using the data for water will be applied to other fluids, in particular, CO_2 which is of current interest for supercritical extraction.

A further study will also be made of the joining of scaling-law formulations for the critical region with classical formulations for the remainder of the PT surface.

CATION-NITROGEN DISTANCE IN NITRIDES OF CRYSTALLINE COMPOUNDS

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

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

CRYSTALLOGRAPHIC DATA FOR ORGANIC MATERIALS

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

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

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

FUNDAMENTAL PHYSICAL CONSTANTS

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

Fundamental Physical Constants are those quantities which provide the foundation of our understanding of the physical universe. This project has concerned itself with two important aspects in the analysis of these constants: the "best" values, which are so important for science and technology, in general, and discrepancies among the constants, which are important in defining new measurement needs or improvement in theory or experiment. A part of this effort is the continuing compilation of data for the 1983 adjustment by a CODATA Task Group.

MOLECULAR STRUCTURE AND THERMODYNAMIC PROPERTIES OF ALKALI METAL VAPORS

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

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

OSRD BINARY PHASE DIAGRAM EVALUATION PROJECTS

Rare Earth Alloys

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

Copper Alloys

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

Vanadium and Niobium Alloys

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

Titanium Alloys

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

Alkali Metals

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

Chromium Alloys

J. P. Neumann
University of Alabama
University, Alabama
Source of Support: DOE

These evaluation projects are a major part of the National Bureau of Standards-American Society of Metals (ASM) joint program to provide reliable phase stability information to the U.S. materials community. The format of all projects is the same. For each binary system a recommended phase diagram will be produced with explanatory text including evaluation of available experimental, crystallographic, and thermodynamic data. The outputs will be published first in the Bulletin of Alloy Phase Diagrams and, as larger numbers of systems are completed, in a series of monographs published by ASM.

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

REFERENCE DATA ON THE REFRACTIVE INDEX OF SELECTED OPTICAL MATERIALS

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

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

ESCA DATA BASE PROJECT

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

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

CORROSION RATE DATA FOR STAINLESS STEEL

M. Marek
Georgia Institute of Technology
Atlanta, Georgia
Source of Support: NBS

This is a pilot project in the NBS/NACE corrosion data program. The objective is to compile and evaluate corrosion rate data for austenitic stainless steels in aqueous chloride solution and to organize the data in

suitable formats for presentation and retrieval. An important part of this effort is to identify the parameters which are important for the evaluation of corrosion susceptibility of these steels.

THERMODYNAMIC REFERENCE DATA OF ELEMENTS AND BINARY ALLOYS

Pramod D. Desai
CINDAS
Purdue University
West Lafayette, Indiana
Source of Support: NSF

A key component of the NBS/ASM phase diagram evaluation program is the use of modeling software to ensure thermodynamic consistency. This project focuses on compiling and evaluating the thermodynamic data for a selected number of elements and alloys for use by evaluators in the NBS/ASM program. It will initially concentrate on Fe, Al and Ti alloys.

STANDARDS FOR COMPUTERIZATION OF MECHANICAL PROPERTY DATA

Jack Westbrook
General Electric
Schenectady, New York
Source of Support: Army

The move towards providing computer access to materials data such as mechanical properties has led to some potential problem caused by the ease with which computers can combine data from different sources. This project is examining these problems for a few mechanical properties of a small number of materials. The result will be a set of recommendations for new procedures and standards which can be the basis of broader activities by U.S. engineering standards groups and NBS.

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

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

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

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

An Annotated Compilation and Appraisal of Electron Swarm Data in Electronegative Gases
J. W. Gallagher, E. C. Beaty, J. Dutton, and L. C. Pitchford

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

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

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

Energy Levels of Silicon, Si I through Si XIV
W. C. Martin and Romuald Zalubas

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

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

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

Erratum: Viscosity of Water Substance - New International Formulation and Its Background
A. Nagashima

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

Small-Angle Rayleigh Scattering of Photons at High Energies: Tabulations of Relativisitic HFS Modified Atomic Form Factors
D. Schaupp, M. Schumacher, F. Smend, P. Rullhusen, and J. H. Hubbell

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

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

Molten Salts: Volume 5, Part 2. Additional Single and Multi-Component Salt Systems. Electrical Conductance, Density, Viscosity and Surface Tension Data
G. J. Janz and R. P. T. Tomkins

International Tables of the Surface of Water
N. B. Vargaftik, B. N. Volkov and L. D. Voljak

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

Evaluated Theoretical Cross Section Data for Charge Exchange of Multiply Charged Ions with Atoms. II. Hydrogen Atom-Partially Stripped Systems
J. W. Gallagher, B. H. Bransden, and R. J. Janev

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

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

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

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

Vapor Pressures of Coal Chemicals
J. Chao, C. T. Lin, and T. H. Chung

NSRDS-NBS Series

Selected Tables of Atomic Spectra: A. Atomic Energy levels - Second Edition; B. Multiplet Tables; O IV
Charlotte E. Moore
NSRD-NBS3(10)

Other Publications in NBS Series

Technical Activities, Office of Standard Reference Data
Sherman P. Fivozinsky
NBS IR83-2661

Electrical Properties of Interfaces - Compilation of Data on the Electrical Double Layer on Mercury Electrodes
J. Lyklema and R. Parsons
NBS IR83-2714

Data Publications from Other Publishers

Manual for Predicting Chemical Process Design Data
Data Prediction Manual
Design Institute For Physical Property Data,
American Institute of Chemical Engineers,
R. P. Danner, and T. E. Daubert

Bibliographies and Indexes from Other Publishers

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Vol. 16. 1983
Radiation Chemistry Data Center

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Vol. 15. 1982
Radiation Chemistry Data Center

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

Machine Readable Data Bases

Thermophysical Properties of Helium
Magnetic Tape 5
Magnetic data tape available from the Office of Standard Reference Data

Interactive Fortran Program to Calculate Thermophysical Properties of Six Fluids
Magnetic Tape 6
Magnetic data tape available from the Office of Standard Reference Data

PUBLICATIONS SCHEDULED FOR 1984

Journal of Physical and Chemical Reference Data, Volume 13

JANAF Thermochemical Tables, Third Edition
M. W. Chase, Jr., Editor

Heat Capacities, Entropies and Some Phase Transition Properties of Organic Compounds in the Liquid and Solid Phases
Eugene S. Domalski, William H. Evans, and Elizabeth D. Hearing

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

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

Refractive Index of ZnS, ZnSe, and ZnTe and Its Wavelength and Temperature Derivatives
H. H. Li

Differential Cross Sections for Elastic Scattering of Electrons by Atomic Targets: I. Experimental Data for Helium and Atomic Hydrogen
J. A. Rees, E. C. Beaty, and J. W. Gallagher

Definition of Recommended Values of Certain Thermodynamic Properties for the Ketones
Buford D. Smith and Ol Muthu

Water Solubility and Related Parameters of Coal Derived Compounds
Sujit Banerjee

High Temperature Vaporization Behavior of Oxides: I. Alkali Metal Binary Oxides
R. H. Lamoreaux and D. L. Hildenbrand

Thermodynamic Properties of Aqueous Sodium Chloride Solutions
K. S. Pitzer, J. C. Peiper, and R. H. Busey

Electrical Resistivity of Chromium, Cobalt, Iron, and Nickel
T. K. Chu and C. Y. Ho

Thermodynamic and Transport Properties of the Noble Gases and Their Mixtures
J. Kestin, E. Knierim, E. Mason, B. Najafi, S. Ro, and M. Waldman

Representative Equations for the Viscosity of Water Substance
J. V. Sengers and B. Kamgar-Parsi

Thermophysical Properties of Fluid H_2O
J. Kestin, J. V. Sengers, B. Kamgar-Parsi, and
J. M. H. Levelt Sengers

Electrical Resistivity of Aluminum and Manganese and Electrical Resistivity of Vanadium and Zirconium
P. D. Desai, H. M. James, and C. Y. Ho

Atlas of the Schumann-Runge Absorption Bands of O_2 in the Wavelength Region 175-205 nm
K. Yoshino, D. E. Freeman, and W. H. Parkinson

Experimental Stark Width and Shifts for Non-Hydrogenic Spectral Lines of Ionized Atoms (A Critical Review and Tabulation of Selected Data)
N. Konjevic , M. S. Dimitrijevic and W. L. Wiese

Evaluated Theoretical Cross Section Data for Charge Exchange of Multiply Charged Ions with Atoms. III. Non-Hydrogenic Target Atoms
R. K. Janev and J. W. Gallagher

Microwave Spectra of Molecules of Astrophysical Interest. XXII. Sulfur Dioxide (SO_2)
F. J. Lovas

NSRDS-NBS Series Publications Scheduled for 1984

Selected Tables of Atomic Spectra: A. Atomic Energy Levels - Second Edition; B. Multiplet Tables; O III
Charlotte E. Moore
NSRD-NBS3(11)

Data Publications Scheduled from Other Publishers in 1984

Medical Linear Accelerator Central Axis Depth-Dose Data
James A. Purdy, William B. Harms, and
Sherman P. Fivozinsky

NBS/NRC Steam Tables, Thermodynamic and Transport Properties and Computer Programs for Vapor and Liquid States of Water
Lester Haar, John S. Gallagher, and George S. Kell
Hemisphere Press

Bibliographies and Indexes Scheduled from Other Publishers in 1984

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Vol. 17. 1984
Radiation Chemistry Data Center

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Vol. 16.1983
Radiation Chemistry Data Center

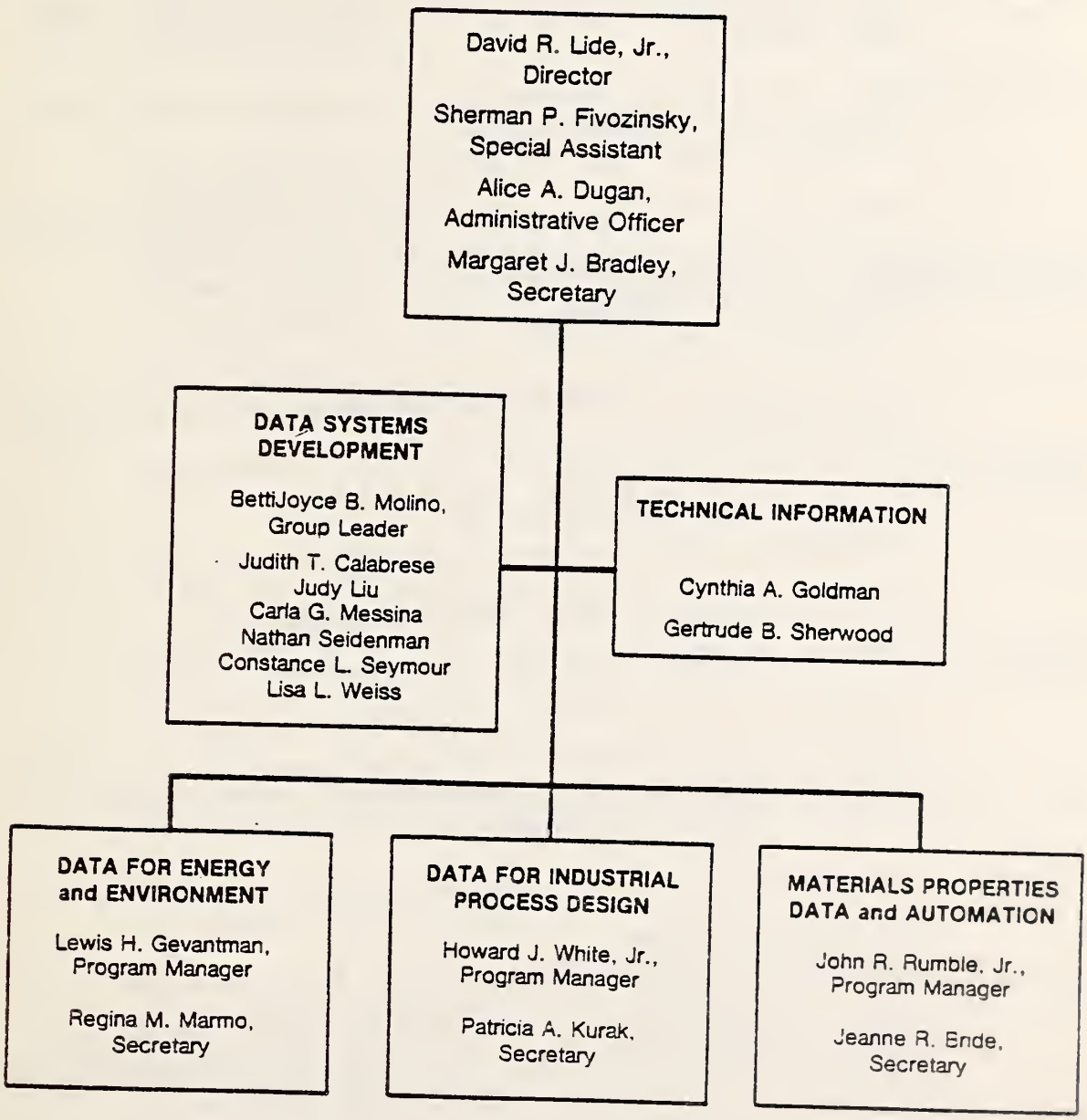
Bulletin of Chemical Thermodynamics, Volume 27, 1984
IUPAC Commissiion on Thermodynamics and Thermochemistry,
Robert D. Freeman, Editor

LIST OF ACRONYMS AND ABBREVIATIONS

AAAS	American Association for the Advancement of Science
AAPM	American Association of Physicists in Medicine (AIP)
ACerS	American Ceramic Society
ACS	American Chemical Society
ADP	Automatic data processing
AGARD	Advisory Group for Aerospace Research and Development
AIAA	American Institute of Aeronautics and Astronautics
AIChE	American Institute of Chemical Engineers
AIME	American Institute of Mining, Metallurgical, and Petroleum Engineers
AIP	American Institute of Physics
API	American Petroleum Institute
APS	American Physical Society
ASM	American Society for Metals
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
BAPD	Bulletin of Alloy Phase Diagrams
BRS	Bibliographic Retrieval Services, Inc.
BWR	Benedict-Webb-Rubin (formulation)
CAC	Center for Analytical Chemistry, NML, NBS
CAD	Computer-Aided Design
CAM	Computer-Aided Manufacturing
CAPQ	Center for Absolute Physical Quantities, NML, NBS
CAS	Chemical Abstracts Science
CBS	Center for Basic Standards, NML, NBS
CCE	Center for Chemical Engineering, NEL, NBS
CCP	Center for Chemical Physics, NML, NBS
CINDAS	Center for Information and Numerical Data Analysis and Synthesis, Purdue University
CIS	Chemical Information System (NIH/EPA)
CISTI	Canada Institute for Scientific and Technical Information
CMS	Center for Materials Science, NML, NBS
CODATA	Committee on Data for Science and Technology (ICSU)
CPSC	Consumer Product Safety Commission
CRR	Center for Radiation Research, NML, NBS
CSIN	Chemical Substances Information Network (EPA)
DARPA	Defense Advanced Research Projects Agency
DIPPR	Design Institute for Physical Property Data (AIChE)
DOE	U.S. Department of Energy
EEO	Equal Employment Opportunity
EPA	U.S. Environmental Protection Agency
EPRI	Electric Power Research Institute
ESCA	Electron Spectroscopy for Chemical Analysis
FDA	Food and Drug Administration
FY	Fiscal Year
GPE	General Purpose Equipment
GPSDC	General Purpose Scientific Document Code
GRI	Gas Research Institute
HGK	Haar-Gallagher-Kell (formulation)
HP	Hewlett-Packard
IAPS	International Association for the Properties of Steam
ICPEAC	International Conference on Photon and Electron Atomic Collisions
ICSU	International Council of Scientific Unions

INCRA	International Copper Research Association
IUPAC	International Union of Pure and Applied Chemistry (ICSU)
JANAF	Joint Army, Navy, Air Force (historical acronym)
JCAMP	Joint Committee on Atomic and Molecular Physical Data
JCPDS	Joint Committee on Powder Diffraction Standards
JCPDS-ICDD	JCPDS-International Centre for Diffraction Data
JILA	Joint Institute for Laboratory Astrophysics, NML, NBS-U. of Col.
JPCRD	Journal of Physical and Chemical Reference Data
LLL	Lawrence Livermore National Laboratory
MPC	Metals Properties Council
MS	Mass Spectroscopy
MSDC	Mass Spectral Data Centre (UK)
NACE	National Assocation of Corrosion Engineers
NAS	National Academy of Sciences
NATO	North Atlantic Treaty Organization
NBS	National Bureau of Standards
NCI	National Cancer Institute
NDE	Nondestructive Evaluation
NEL	National Engineering Laboratory, NBS
NIH	National Institutes of Health
NLM	National Library of Medicine
NML	National Measurement Laboratory, NBS
NRC	National Research Council
NSF	National Science Foundation
NSRDS	National Standard Reference Data System
OA	Other Agency (Funding)
ONR	Office of Naval Research
OSRD	Office of Standard Reference Data, NML, NBS
OSRM	Office of Standard Reference Materials, NML, NBS
PDFC	Phase Diagrams for Ceramists Data Center
PL	Public Law
PMS	Physical Measurement Services
RCDC	Radiation Chemistry Data Center
RPI	Rensselaer Polytechnic Institute
SAE	Society of Automotive Engineers
SLAIM	Spectral Line Atlas of Interstellar Molecules
SPE	Society of Plastics Engineers
SRD	Standard Reference Data
SRM	Standard Reference Material
STRS	Scientific and Technical Research and Services (appropriated NBS funds)
TRAPP	Thermophysical Properties of Hydrocarbon Mixtures Database
UNESCO	United Nations Educational, Scientific, and Cultural Organization
USGS	United States Geological Survey

OFFICE OF STANDARD REFERENCE DATA



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PUBLICATIONS BY OSRD STAFF

NBS/EPA/NIH Mass Spectral Data Base, Supplement 2, 1983, S. R. Heller, G. W. A. Milne, and L. H. Gevantman, NSRDS-NBS 63, Suppl. 2

Computerized Materials Data Systems, J. H. Westbrook and J. R. Rumble, Jr., Editors, A Report of a Workshop (1983)

State-to-State Differential Cross-Sections for Vibrational-Rotational Excitation and Elastic Scattering of Electrons by N_2 at 5-50 eV: Calculations Using Extended-Basis-Set Hartree-Fock Wavefunctions, J. R. Rumble, Jr., D. G. Truhlar, and M. A. Morrison, J. Chem. Phys. 78 (1983)

Status and Trends of Numeric Data Banks and Systems, J. Rumble, Jr., Proc. 8th CODATA International Conference, Pergamon Press (1983)

Chemical Thermodynamics in Steam Power Cycles Data Requirements, Howard J. White, Jr. and Otakar Jonas, Editors, Proceedings of a Workshop held at NBS, February 8-9, 1983

INVITED TALKS AND PRESENTATIONS BY OSRD STAFF

Introductory Remarks (Chairman), Symposium on Numerical Data Quality, American Chemical Society Annual Meeting, Washington, DC, August 1983
Lewis H. Gevantman

Numerical Data Dissemination: Past, Present, and Future, Chemical Abstracts Service, Columbus, OH, April 1983
David R. Lide, Jr.

The National Standard Reference Data System of the United States, European Summer School on Computing Techniques in Physics, Bechyne, Czechoslovakia, June 1983
David R. Lide, Jr.

Remarks on the History of CODATA, Conference on CODATA Future, La Gaillarde, France, June 1983
David R. Lide, Jr.

The CODATA Role in International and Interdisciplinary Cooperation, European Summer School on Computing Techniques in Physics, Bechyne, Czechoslovakia, June 1983
David R. Lide, Jr.

Overview of Numerical Data Bases, NATO/AGARD Lecture Series on Development and Use of Numerical and Factual Data Bases, Gaithersburg, Md.; London, England; and Lisbon, Portugal, October 1983
David R. Lide, Jr.

The State of the Art on Numerical Data Bases, UNESCO Training Course on Accessibility & Dissemination of Data in Science & Technology, Stockholm, Sweden, October 1983
David R. Lide, Jr.

New Modes of Reference Data Dissemination, U.S.-Japan Joint Seminar on Thermophysical Properties, Tokyo, Japan, October 1983
David R. Lide, Jr.

Validation of Data on Materials Properties, American Society of Mechanical Engineers Winter Meeting, Boston, Mass., November 1983
David R. Lide, Jr.

Introductory Remarks (Chairman), Symposium on Numerical Data Dissemination, American Chemical Society Annual Meeting, Washington, DC, August 1983
Bettijoyce B. Molino

"Vibrational-Rotational Excitation of N_2 by Electrons at 5-50 eV," XIII ICPEAC Meeting, Berlin, FRG, August 1983
John R. Rumble, Jr.

"Electron Scattering by N_2: Calculations Using MCSCF Target Wavefunctions," XIII ICPEAC Meeting, Berlin, FRG, August 1983
John R. Rumble, Jr.

"Numeric Data Bases in Science and Technology," American Chemical Society Annual Meeting, Washington, DC, August 1983
John R. Rumble, Jr.

The concept of non-bibliographic data in different areas with applications to R&D and practice. C. Physics related areas, CODATA Seminar on Non-Bibliographic Data Banks, Stockholm, Sweden, October 1983
John R. Rumble, Jr.

Planning and designing numerical database systems in science and technology, CODATA Seminar on Non-Bibliographic Data Banks, Stockholm, Sweden, October 1983
John R. Rumble, Jr.

IAPS and ASME Research Committee on the Properties of Steam, Workshop on Thermodynamics in Steam Power Cycles Data Requirements, NBS, Washington, DC, February 1983
Howard J. White, Jr.

Chemical Thermodynamics in Steam Power Systems - Data Requirements, 44th International Water Conference, Pittsburgh, Pa., October 24-26, 1983
Howard J. White, Jr. (with Otakar Jonas)

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

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Council of the American Physical Society (APS)

Audit Committee, APS (Chairman)

Committee on Fellowships, Division of Chemical Physics, APS

1983 Irving Langmuir Prize Committee, APS (Chairman)

American Institute of Physics (AIP) Publication Board

Committee on Nomenclature, ACS

Division of Physical Chemistry, ACS (Alternate Councilor)

Chemical Abstracts Advisory Board, ACS

Section Committee, Chemistry, AAAS

Petroleum Research Fund Advisory Board, ACS

Journal of Physical and Chemical Reference Data (Editor)

Committee on Data for Science and Technology of International Council of Scientific Unions (Secretary-General)

CODATA Publication Committee (Chairman)

CODATA Bulletin (Associate Editor)

Program Committee for Eighth International CODATA Conference

Joint Committee on Atomic and Molecular Physical Data (JCAMP)

Interdivisional Committee on Nomenclature and Symbols, IUPAC

Commission on Symbols, Terminology, and Units, IUPAC

Physical Chemistry Division, IUPAC (President-Elect)

Chemical Information System (CIS) Steering Committee (Chairman)

NAS/NRC Committee on Atomic and Molecular Science

Lewis H. Gevantman

IUPAC Commission V.8 on Solubility Data (Secretary)

Executive Committee, Joint Committee on Atomic and Molecular Physical Data

Subcommittee on the Chemical Substance Information Network (CSIN)

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

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

CIS Management Advisory Board (Chairman)

Interagency Toxic Substance Committee (Observer)

Howard J. White, Jr.

International Association for the Properties of Steam (Executive Secretary)

Task Group on Chemical Thermodynamic Tables (CODATA/ICSU) (Chairman)

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

Engineering Sciences Data Unit Ltd. (Corresponding Member)

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

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

American Petroleum Institute Subcommittee on Technical Data (Advisor)

John R. Rumble, Jr.

Organizing Committee, Materials Data Workshop, Fairfield Glade, Tennessee

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Management Board, NBS/JCPDS-International Centre for Diffraction Data, Cooperative Program

Steering Committee, NACE/NBS Program on Corrosion Data

ASME Task Force on Materials Data for Elevated Temperature Design and Analysis

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

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Bettijoyce B. Molino

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Alice A. Dugan

NML Administrative Council

NML-EEO Women's Personnel Panel, NBS

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. 61 Stat. 655; 76 Stat. 446.

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

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

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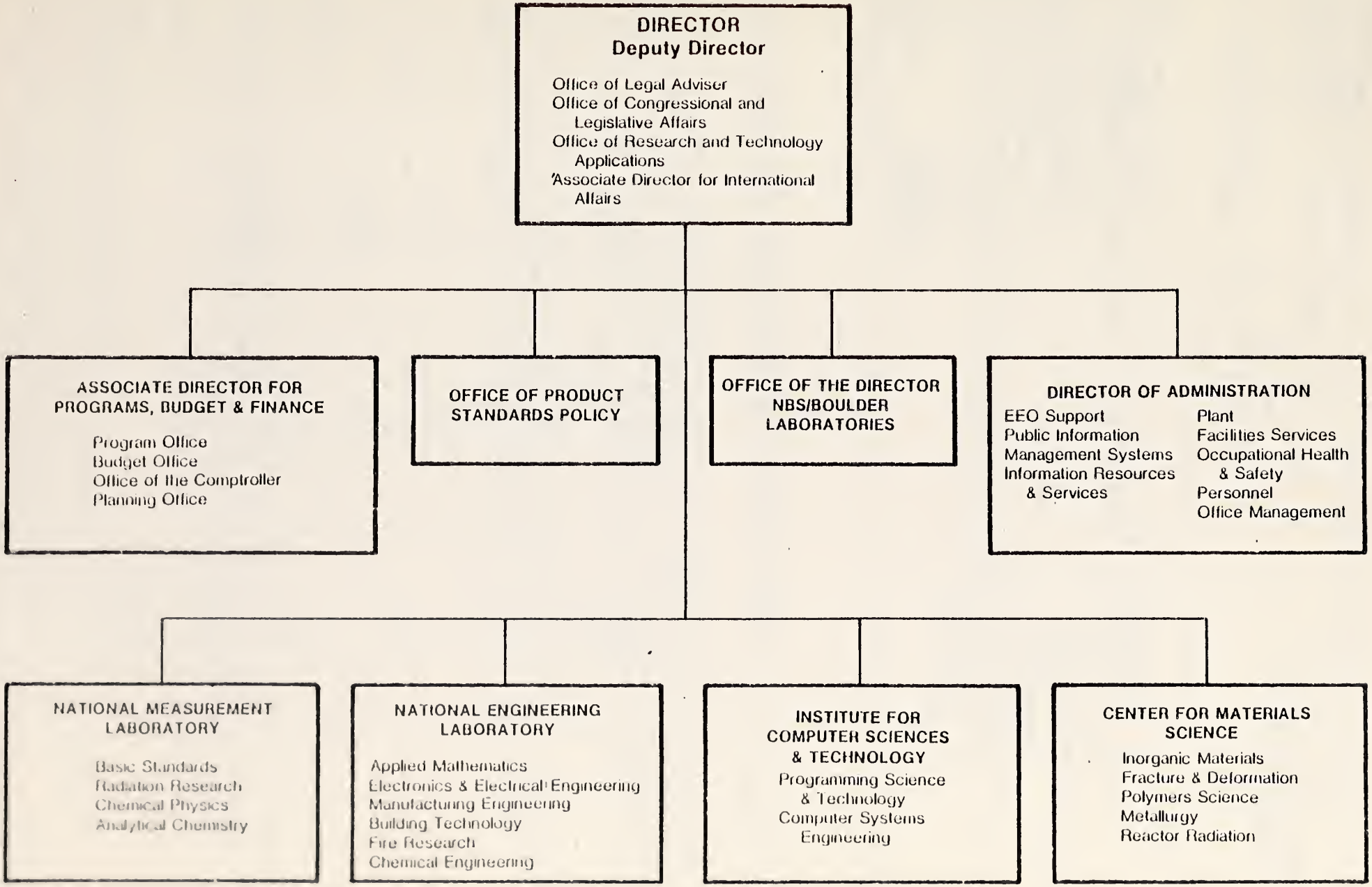
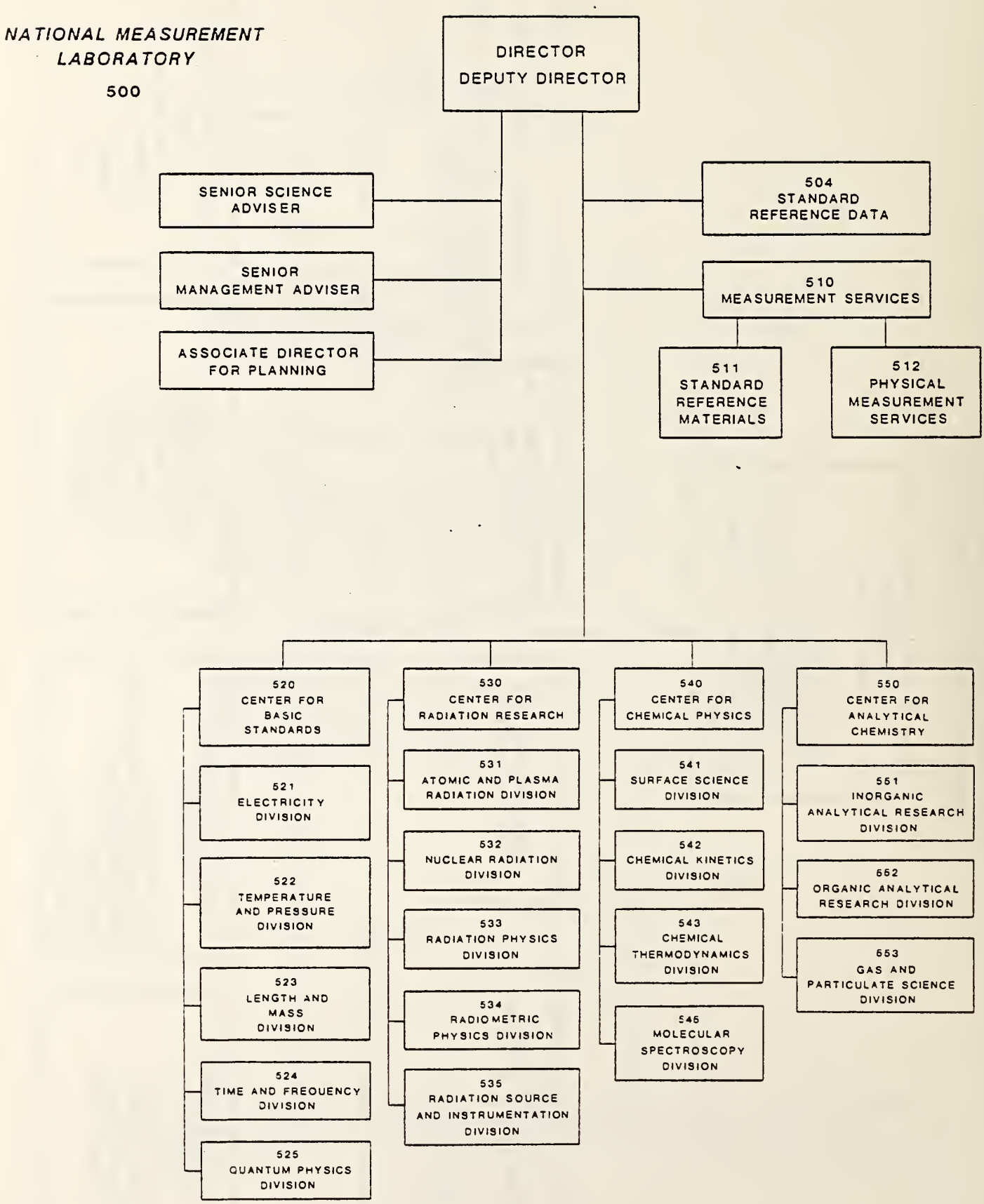
National Bureau of Standards

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WASHINGTON, D.C. 20234

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9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP)

10. SUPPLEMENTARY NOTES

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

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

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

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1983.

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

data compilation; energy and environmental data; evaluated data; materials data; standard reference data; technical activities 1983; thermochemical and thermophysical data

13. AVAILABILITY

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