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# T Technical Activities 1985

Office of  
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National Bureau of Standards



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# T Technical Activities 1985

## Office of Standard Reference Data

Sherman P. Fivozinsky, Editor

**U.S. DEPARTMENT OF COMMERCE**  
**National Bureau of Standards**  
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**U.S. DEPARTMENT OF COMMERCE**, Malcolm Baldrige, Secretary  
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## ABSTRACT

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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 databases of critically evaluated physical, chemical, and materials properties of substances. These databases are available through NBS and private publications, on magnetic tape, and from online 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 1985.

Key words: chemical data; data compilation; evaluated data; materials properties data; numerical database; physical data; standard reference data; technical activities 1985.

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## INTRODUCTION

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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 border-line 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:

National Standard Reference Database Series - Computer-readable databases available in standard magnetic tape format under lease arrangements.

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, online networks, and other computer-based formats.

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



## PROGRAM STRUCTURE

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Current activities in the Standard Reference Data program are carried out in 23 data centers and approximately 40 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 discipline-oriented program areas:

Physical Data - Includes data on atomic, molecular, and nuclear properties, and spectral data utilized for chemical identification.

Chemical Data - Covers primarily kinetic, thermodynamic, and transport properties of substances important to the chemical and related industries.

Materials Properties Data - Includes structural, electrical, optical, 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 for 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:

<u>Series</u>	<u>Publications in 1985</u>	
	<u>Pages Published</u>	<u>Titles Published</u>
JPCRD, Vol. 14	3586	25
Data Compilations from other publishers		
Other Publications in NBS Series	545	5
Bibliographies and indexes from other publishers	1541	3
	<hr/>	<hr/>
Totals	5672	33

Subscribers to JPCRD

<u>Month/Year</u>	<u>Number</u>
9/1981	1265
9/1982	1234
9/1983	1230
9/1984	1186
9/1985	1160

Inquiries Received in OSRD

(Does not include inquiries received by data centers)

<u>Year</u>	<u>Number</u>
1981	657
1982	613
1983	1022
1984	616
1985	623

Sales of JPCRD Offprints and Supplements

<u>Year</u>	<u>Offprints</u>	<u>Supplements</u>
1981	4254	137
1982	3567	266
1983	3081	1666
1984	2900	1300
1985*	3180	547

\*Projected to end of year

S. P. Fivozinsky, Program Manager

The Physical Data Program was created last year as the result of a change in the technical management structure within OSRD. The old programmatic areas, Energy and Environmental Data, and Industrial Process Data, were reorganized to reflect a disciplinary content rather than application areas. As a result, the new Physical Data Program is concerned with atomic, molecular, nuclear, and those spectral databases used heavily in analytical chemical instrumentation. The following data centers are associated with the Physical Data Program.

- \* Atomic Collisions Cross Section Data Center (CBS, JILA)
- \* Atomic Energy Levels Data Center (CRR)
- \* Atomic Transition Probabilities Data Center (CRR)
- \* Fundamental Constants Data Center (CBS)
- \* Molecular Spectra Data Center (CCP)
- \* Photon and Charged Particle Data Center (CRR)

These data centers are long-term activities which develop, maintain, and disseminate a major database in these areas. The Physical Data Program also supports a number of short-term projects whose efforts lead to specific one-time outputs. The following projects have been active during this calendar year:

- \* Critical Compilation of Mass Spectral Data
- \* Compilation of Atomic Wavelengths below 2000 Å
- \* K shell Ionization by Hydrogen and Helium Ions
- \* Digitization of the Coblenz Society Infrared Database
- \* Soft X-ray Interactions with Matter
- \* Medical Physics Data Book, 2nd edition
- \* Atomic Transition Probabilities for Energy Research
- \* Spectroscopic Properties of Excited Electronic States of Small Polyatomic Transient Molecules
- \* Critical Compilations and Reviews of Data Describing the Electron Impact Excitation of Atoms and Atomic Ions
- \* Mass Spectral Database Project

Through the combination of data centers and short-term projects the Physical Data Program addresses the most critical needs for databases with a combination of NBS and other-agency funding. More detailed descriptions of the data centers, the short-term projects, and their current activities and future plans, are found later in this report.

While most outputs of the Program are in printed form, an increasing number of computer-readable databases are being designed and disseminated. In the future, internal operations of data centers, evaluation techniques, and dissemination will involve heavy utilization of modern computer technology.

## HIGHLIGHTS OF RECENT ACTIVITIES

### New Interagency Agreement with EPA

The National Bureau of Standards and the Environmental Protection Agency have signed an Interagency Agreement which provides for joint management of the NBS/EPA/NIH/MSDC Mass Spectral Database. In addition, the agreement includes the future development of an infrared spectral database.

The Mass Spectral Database is a major international chemical identification resource. It is leased from the Office of Standard Reference Data in computer-readable form and sold as a set of seven books. It is utilized by scientists in industry, government, and universities in printed form, on their institutions' computer systems, through online retrieval services, and through use of hundreds of mass spectrometer systems which are sold with a copy of the database and built-in search software.

Under the agreement, the EPA Environmental Monitoring and Support Laboratory in Cincinnati, Ohio carries out acceptance and insertion of new spectra, applies quality control procedures to the file, and generates periodic updates to the database. The Office of Standard Reference Data sponsors the collection of new spectra, establishes criteria for evaluation of the spectra, arranges for dissemination of printed and computer-readable versions of the file, and manages the revenues resulting from lease or sale of the database and the reinvestment of those funds in the further development of the system. The long-term nature of this effort may dictate the establishment of a new Mass Spectral Data Center within the Physical Data Program. OSRD supports part of the EPA/Cincinnati effort.

The agreement also called for the establishment of an advisory committee to provide review of project activities. Five well-known scientists have accepted membership. They are: Dr. Charles Anderson, Nicolet Analytical Institute, Dr. Robert Finnigan, Finnigan Instruments, Dr. Jeanette Grasselli, Standard Oil of Ohio, Dr. Milton Levenberg, Abbott Laboratories and Dr. Charles Wilkins, University of California. The members of the Committee are expert in both mass and infrared spectral data measurement and use. They will meet once each year to review activities of the Project and to make recommendations. The first meeting of the group will probably take place in the winter, 1985/86.

The new Mass Spectral Data Project has already issued an update of the Mass Spectral Database. The database now contains 42,261 electron impact mass spectra, an increase of 2434 over the previous version. The Mass Spectral Data Project also depends on receiving new mass spectra from the Mass Spectrometry Data Centre (MSDC) in Nottingham, England. We are presently negotiating a new Memorandum of Understanding with the Royal Society of Chemistry, which operates the Nottingham Data Center.

We are also beginning to prepare a new printed edition of the Mass Spectral Database. Camera-ready copy will be prepared with the assistance of Chemical Abstracts Service in Columbus, Ohio.

## Databases

Two computer-readable databases, EPSTAR and XGAM, have been added to the NBS Standard Reference Database Series. EPSTAR provides electron and positron stopping powers of materials in an energy range from 10 keV to 10 GeV. Electron stopping powers can be obtained for 285 materials, and positron stopping power information is available in 29 materials. XGAM provides photon attenuation cross sections for the elements along with interactive software which calculates attenuation coefficients in any complex substance defined by the user. The XGAM energy range is from 1 keV to 100 GeV.

During the past year, the Coblenz Society Evaluated Infrared Data Compilation was being digitized. A computer-readable database of over 4,100 digitized spectra has been delivered. We plan to make these data available through cooperation with the Fachinformationszentrum in Karlsruhe, West Germany.

A major compilation of atomic wavelengths below 2000 Å is being prepared for publication. It will constitute a two-volume supplement to the Journal of Physical and Chemical Reference Data. In addition, because the compilation resides in its entirety in a computer file, it may, at some future time, also be released as a computer-readable database.

## New Projects

Two new projects have begun this year with other-agency funding; these are in addition to the new Mass Spectral Data Project. Dr. Jean Gallagher of the University of Colorado will carry out critical compilations and reviews of data describing the electron impact excitation of atoms and atomic ions. Dr. Marilyn Jacox of NBS will compile and evaluate spectroscopic properties of excited electronic states of small polyatomic transient molecules.

## Data Centers

The Atomic Energy Levels and Atomic Transition Probabilities Data Centers are presently working on the development of a major database management system for atomic structural data. The system should be complete and in use within a year. Considerable interest in this system and its implications for the availability of atomic structural data in computer-readable forms has been expressed by the scientific community through, for example, the NAS/NRC Committee on Line Spectra of the Elements, and members of the NAS/NRC Board on Assessment for the National Bureau of Standards.

The Fundamental Constants Data Center is completing the "1985 Least Squares Adjustment of the Fundamental Constants." This effort represents the primary source of information in the world on the values of the fundamental physical constants. The new set of recommended values will be published as a CODATA Bulletin in early 1986. The full details of the adjustment will be submitted for separate publication later that year.

The Atomic Collisions Cross Section Data Center at JILA in Boulder, Colorado, has been preparing a computerized database of electron collision cross sections with atoms, ions, and molecules. These data are important in modelling gas discharges and plasma systems such as those describing nuclear fusion processes and interstellar atmospheres. At the present time about 900 numerical data files have been entered into the database. These are being used to prepare figures supporting the Center's review activities. Programs are being developed to produce listings and indices of the material in the database and to provide an online inquiry capability.

The Molecular Spectra Data Center is publishing a compilation of recommended rest frequencies of interstellar molecular transitions in the microwave region. Earlier this year, the microwave spectrum of sulfur dioxide was published as part 22 of the well known series "Microwave Spectra of Molecules of Astrophysical Interest." Microwave spectral data are the key to analyses of interstellar data coming from radio-telescopes.

The Photon and Charged Particle Data Center has had a long and successful history of providing photon and electron interaction cross section and radiation transport data for varied applications in medicine, health physics, and national defense. This year the Center released two interactive computer-readable databases. EPSTAR provides electron and positron stopping power data (285 materials for electrons, 29 materials for positrons). XGAM calculates photon interaction cross sections and attenuation coefficients on whatever substance the user inputs.

H. J. White, Jr. Program Manager

The program on chemical data is concentrated in the areas of thermodynamics, transport properties and chemical kinetics. These are areas where reference data are most frequently needed both for scientific and industrial use, especially in the chemical, petrochemical and petroleum refining industries. Also, these areas compliment those covered in other parts of the program, particularly, materials data.

Two characteristic traits of the program will be given special attention. They are: automation and cooperative projects. The obvious powers of the computer in data-base management gave it its initial impetus into the reference data field and the development of various automated products has followed closely. The desirability of commonly agreed-upon data bases in many areas and a general shortage of resources have led to a number of cooperative projects. More will be said on both subjects throughout this report.

A major part of the thermodynamic effort involves chemical thermodynamic data. These include enthalpies and Gibbs energies of formation from the elements in their standard states at 298.15K as well as entropies and heat capacities at 298.15K for pure substances and components in solution. Steps are taken to assure that this body of data is thermodynamically consistent. Data for some 14,000 pure substances and aqueous solutions, primarily inorganic, are available in printed tables and in magnetic tape form. Data on the activity and osmotic coefficients at 298.15K for several hundred aqueous electrolyte solutions are also available in printed tables and in an interactive computer version. Efforts are underway to expand these data bases to accommodate more organic substances and cover a wider range of temperatures.

The thermochemistry of substances containing carbon, hydrogen and oxygen and up to four carbon atoms is being systematically studied and a large database on the heat capacities of organic compounds have been published. It exists in automated form but is not yet suitable for release. An automated database on enthalpies of formation has also been purchased.

To expand coverage of temperature, thermal functions for pure substances and aqueous solutions are being developed. The latter task, in particular, requires the development of new techniques.

Turning away from chemical thermodynamics there is an extensive effort on the equations of state and related thermodynamic properties of pure fluids. Also, equations for the viscosities and thermal conductivities of these fluids are prepared which use the densities given by the equations of state so that a consistent set of thermodynamic and transport properties exist. The same set of equations has been used for six fluids so that changing from one fluid to another merely involves changing a set of coefficients. The data and the computer program have been published and an interactive tape version is also available. Data for five more fluids, treated in a similar fashion, will be published shortly. Formulations for other fluids have been prepared using different

equations. An interactive computer program has also been developed which predicts the density and transport properties of a group of fluids, primarily hydrocarbons, over a range of temperatures and pressures using corresponding-states techniques. This program is being improved and expanded to include thermodynamic properties and a wider range of fluids.

The densities, viscosities, electrical conductivities and surface tensions of molten salts, as well as special properties such as the eutectic points of binary systems present another area in which there has been extensive publication of evaluated data and for which an automated data base exists.

The kinetics program is focussed on homogeneous gas-phase kinetics and radiation chemistry including photochemistry. Two major areas of gas-phase kinetics have been concentrated on: atmospheric chemistry and combustion. The atmospheric program, initially principally stratospheric, is part of a large program sponsored by several agencies. Data sheets for 206 rate constants for reactions involving 105 species are available in printed form. For combustion, a data base for 550 reactions involving some 50 odd species has been developed but has not yet been published.

A program bridging kinetics and thermodynamics involves ion kinetics and energetics. The ionization potentials, appearance potentials, and heats of formation of gaseous ions are compiled and evaluated. An extensive database on positive ions is being updated and extended to include negative ions as well.

A new and different system for preparing chemical thermodynamic tables is being developed under the aegis of CODATA. This system is highly automated and permits the preparation of consistent tables in a largely decentralized way. As a result, it is possible to consider the production of international tables using the services of experts from all over the world under the direction of the CODATA Task Group on Chemical Thermodynamic Tables. CODATA is publishing two major reports related to this work. One contains formation data for a set of key chemical compounds; the other is a prototype set of the new tables. OSRD and OSRD data centers have played central roles in the production of both of these CODATA publications and in the design and development of the new system for producing international tables.

New evaluated data for the heats of combustion of the lower hydrocarbons and for calculating the heat of combustion of natural gas samples have been prepared by two OSRD data centers on behalf of a number of industrial associations both national and international. These data could become the basis for an international standard.

As befits its importance in science and engineering, water has its own formulations for its thermodynamic and transport properties. At the 10th International Conference on the Properties of Steam, the International Association for the Properties of Steam approved a new formulation for the thermodynamic properties of ordinary water substance for scientific and general use which now is being published around the world. Recently, new formulations for the viscosity and thermal conductivity of ordinary water substance have also been approved. Work done in this program played a major role in the preparation of all of



these formulations. The properties of water are also available on computer tape and steps are being taken to make them available on a diskette for an IBM PC.

Work is also underway to prepare an internationally accepted formulation for the thermodynamic properties of ethylene under the auspices of IUPAC.

OSRD interactions with DIPPR, an activity of the American Institute for Chemical Engineers sponsored by the chemical industry, represent another cooperative venture. This fall, two user cooperative agreements have been signed with AIChE. One extends the previous programmatic cooperation between OSRD and DIPPR. The second establishes cooperation in disseminating the new DIPPR database in computer-readable form.

## MATERIALS PROPERTIES DATA

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J. R. Rumble, Jr., Program Manager

The past year has been one of continuing growth for the Materials Properties Data Program. Highlights include the start of a prototype of a computerized materials data system, major compilations of evaluated data, and new data evaluation activities. The program has five components as shown in Table 1. In each area, projects are underway and new activities are planned, depending on funding.

Table 1

---

OSRD Materials Properties Data Program
Structure and Characterization
Physical Properties
Phase Equilibria
Performance Properties
Corrosion
Mechanical Properties

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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. 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.

Table 2

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

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The Materials Properties Data Program has a number of short-term evaluation projects that address specific data needs within the framework given in Table 3. These are done 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.

Table 3

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OSRD Materials Properties Data Program

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Structure and Characterization

Crystallography

NBS Crystal Data Center

Evaluation Models for Powder Diffraction Data - JCPDS-ICDD

Cambridge Crystallographic Data Centre

Cation-Nitrogen Distance - University of Illinois - Chicago

Surfaces

ESCA Data Project - Surfax (CA)

Ion Sputtering - NBS

Low-Energy Electron Diffraction - Oregon State University

Physical Properties

Molecular Weight of Polymers - NBS

Properties of Glassy-Forming Melts - Alfred University

Phase Equilibria

Alloys

NBS Alloy Phase Diagram Data Center

NBS/ASM Phase Diagram Program

Fe, Al, Ti - NBS

V, Nb - Ames Laboratory

Cr - University of Alabama

Cu - Carnegie-Mellon University

Rare Earths - Iowa State University

Alkalis - Thermfact, Montreal

Actinides - LASL

Ceramics

NBS Phase Diagrams for Ceramists Data Center

Modeling of Complex Ceramic Phase Equilibria - Penn State University

Thermochemistry

Thermochemistry of Alloy and Elements - CINDAS, Purdue University

Corrosion

NBS Corrosion Data Center

NBS/NACE Corrosion Data Program

Stainless Steels in Aqueous Chlorides - Georgia Tech

Crevice Corrosion of Stainless Steels - LaQue Center - North Carolina

Mechanical Properties

Fracture Toughness - NBS

Fatigue - John Deere and SAE

Creep Rupture - Metal Properties Council

Ductile Fracture Toughness of Low-Alloy Steels - University of Florida

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Finally, a major part of the program is to help user groups define their evaluated data needs, set up programs to address them, and find necessary support. In the past year several such efforts have taken place, 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 are 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. The NBS Data Center interaction with the International Centre for Diffraction Data-JCPDS (ICDD-JCPDS) continues. This past year the ICDD-JCPDS has had a research associate at the NBS center working on software to be used with the NBS Crystal Data Identification File. That software is now being distributed by the ICDD-JCPDS with the NBS Crystal Data File.

Surfaces as well as bulk materials have received a great deal of attention. Over the last 20 years, a number of techniques involving electron and photon spectroscopies have been developed to characterize surfaces, and the data generated are in need of evaluation. Projects on ESCA and LEED data are underway. The Surface Science Division in the Center for Chemical Physics has established a project on ion sputtering data.

### Physical Properties

Three manuscripts on evaluating molecular weight data for polymers have been published. In addition, a new effort on the properties of glassy-forming melts has been started.

### Phase Equilibria

NBS, through the Institute for Materials Science and Engineering (IMSE) and OSRD, has two major programs for evaluating phase data for alloys and ceramics. These major programs are well integrated into the user communities, and significant progress was achieved this year.

The Alloy Phase Diagram Center is the focal point of the NBS/American Society for Metals (ASM) joint program to evaluate all alloy phase diagrams. Over the last year, the major thrust was digitizing over 1,000 diagrams for a new publication for binary alloy systems. The Bulletin of Alloy Phase Diagrams published over 50 new diagrams, and work on prototype databases continued. 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 has been implementing their agreement with the American Ceramics Society (ACerS) for a 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.

Phase data for polymeric blends are important in developing new and improved polymers. NBS and the Society for Plastics Engineers (SPE) are awaiting increased availability of funding before proceeding further.

## Performance Properties

### Corrosion

The National Association of Corrosion Engineers (NACE) and NBS are now beginning projects under a cooperative agreement which will provide the technical community with evaluated corrosion data. The Metallurgy Division (IMSE) and OSRD have established the NBS Corrosion Data Center to act as the technical focal point of this program. Several projects have been started in both kinetic and thermodynamic areas. A major corrosion data workshop was held in June and enthusiastically endorsed the proposed evaluation and database building work.

### Mechanical Properties

OSRD has been working closely with outside groups to address a variety of problems related to mechanical properties data. In particular, the Metal 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 five-pronged effort involving a prototype system of data evaluation, data standardization, database creation, and user workshops.

One highlight was the start of a prototype of a comprehensive materials data system, using funding from DOE, DARCOM, NSF, and NBS. The prototype will be available in early 1986.

The evaluation of mechanical properties data until now has been concentrated in areas of high technology such as nuclear power generation and aerospace. This past year, OSRD started several evaluation projects, working with groups such as SAE, MPC, and ASME, as well as individual researchers.

Computer access to mechanical properties data will cause new problems with respect to standardization of data generation and reporting. As a result of the request of NBS and the National Materials Property Data Network, Inc. (NMPDN), ASTM is holding a planning meeting this fall to determine the best standardization activity.

The NMPDN 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 now existing published compilations. NMPDN and OSRD are working together to persuade publishers, societies, and other groups to begin building the needed databases more intensely.

A key ingredient to success in this type of project is strong user input from the beginning. To this end, NBS, working with several groups, has set up a series of user workshops addressing the needs in several application areas. The workshops outline detailed needs and will help pave the way for industrial acceptance and support of the system. In 1985 two workshops were held, one being the Corrosion Data Workshop, and the other the Tribology Data Workshop, held jointly with ASME and DOE. At this workshop, detailed plans for a demonstration tribology information system were developed and will be implemented by DOE and ASME in 1986.

### 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, which OSRD is working to provide. A major effort is continuing to attract from NBS and other government agencies the attention these activities deserve and to turn that attention into direct support.

B. B. Molino, Group Leader

The major commitment by the Office of Standard Reference Data to automate the internal operations of its data centers and to develop numerical databases for dissemination has continued throughout the past year. Progress has been made in many areas, as summarized below.

### Computing Facilities

We are pleased to report that the new Consolidated Scientific Computing System (CS)<sup>2</sup> is now fully operational at NBS. It consists of a CDC Cyber 205 (622 series) supercomputer with a CDC Cyber 180/855 front end and a high-speed loosely coupled network attaching the two. Training has been conducted in all aspects from system overview to operating system procedures to specialized topics such as vector programming. Both OSRD staff and data center personnel have availed themselves of this training and are becoming proficient in using the new facilities.

The OSRD Hewlett Packard 1000 computer facility has been upgraded to an A series machine, giving three times the processing power and better turn-around to the users. We have recently installed a laser printer to enhance the quality of camera-ready scientific material coming from the HP. Several new projects and several additional data centers have begun to use the OSRD facility. In response to this and to aid with our dissemination endeavors, we are procuring two additional 404 megabyte disk drives and an additional tape drive. In addition to providing needed resources to our users, this will allow the Data Systems Development Group to play a more central role in propagating common automation techniques across data centers, to promote standardization and integration whenever possible, and to reduce any duplication of effort. The addition of this hardware is in keeping with our multiyear plan for OSRD computer support facilities. In addition, we have begun to develop our strategy for the future and are researching such additions to our facilities as graphics, the 32 bit word computer which Hewlett Packard will release shortly, the microvax, etc. We continue to coordinate our efforts with the individuals using the HP 1000 in the Center for Chemical Physics, and we continue to increase our library of available software, both purchased and developed in-house.

The office is increasing the number of microcomputers available and now has an Apple, a Hewlett Packard personal computer, an IBM PC, and an IBM XT. Two IBM AT's are on order. We have begun experimenting with downloading the data and software presently available in the NBS Standard Reference Database Series to microcomputers. We anticipate increasing these efforts and discussing alternatives concerning the distribution of Standard Reference Data for personal computers.

Finally, each member of our secretarial staff has received the appropriate training and is now making full use of all the capabilities of word processing equipment. In addition, administrative tasks are being performed on an IBM PC, when appropriate.

### Publication Procedures

The Bedford Composition System for computer typesetting of our publications is operating smoothly. We continue to realize a reduction in the amount of processing required in this office as well as a reduced turn-around time. The manuals we have drafted have proven useful to our users, and even publications from data centers outside NBS are processed with relative ease.

We have begun upgrading this composition system to Bedford's state-of-the-art Vision Network System. The most immediate advantage is the Canon laser printer (CX) which provides considerably better proof copy than the printronix. Other significant advantages include individual stand-alone workstations, each with a 36 megabyte Winchester disk drive, the ability to use IBM PC's as input devices, and the integration of all components via an enhanced ethernet connection.

Also, as part of the Consolidated Scientific Computing System, the laboratory buildings at NBS will have remote printers. The award for these laser printers has been made, and by next year they and such software as TEX will be available to our users.

### Numerical Database Activity

Two new databases have been released in the NBS Standard Reference Database Series. NBS Standard Reference Database 9, called GAMPHI, an interactive FORTRAN program, provides the activity and osmotic coefficients of 350 aqueous electrolyte solutions. Database 10, Thermophysical Properties of Water, also an interactive FORTRAN program, calculates the thermodynamic and transport properties of fluid H<sub>2</sub>O (liquid and vapor) using the formulation as approved by the International Association for the Properties of Steam (IAPS) at its Tenth International Conference in 1984.

All eight NBS Standard Reference Databases presently available (listed in Table 1) have generated considerable interest and a substantial number of leases. Our pricing policy is such that we hope to attract on-line vendors to make the databases available at an acceptable price to traditional user groups in industry, universities, and Government.



Table 1

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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	
9. Activity and Osmotic Coefficients of Aqueous Electrolyte Solutions (GAMPHI)	
10. Thermophysical Properties of Water	

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We anticipate quite a few additions to this NBS Standard Reference Database Series in the near future. Among them will be the JANAF Tables, the DIPPR database, a database of electron and positron stopping powers (EPSTAR), and a database of x-ray and gamma-ray cross sections and attenuation coefficients (XGAM).

We have distributed written instructions to our data centers concerning the preparation of such databases and have formalized the procedures for both the preparation and the distribution of this database series.

We were pleased to be able to demonstrate many of our databases and associated software on Capitol Hill earlier this year to both the Senate staff and the House of Representatives staff as part of "A Look at the National Bureau of Standards."

## Database Activities

Individual data centers continue to make great progress in their database efforts. Ongoing projects in this area are summarized in Table 2.

Table 2

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### OSRD Activities in Numerical Data Bases

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#### 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

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Our major commitment to the automation of the numeric data files for the Atomic Energy Levels Data Center and the Atomic Transition Probabilities Data Center continues. The specification and design of a computerized database system of atomic spectroscopic data is complete, including the description of data elements and their relationships and the design of the file structure. Programs are being developed for entry and validation of new data, editing of existing data, viewing single records, specifying one-dimensional or two-dimensional queries using both keyed and sequential access, and outputting results in intermediate format on either a terminal or a printer.

#### Reference Center Automation

We maintain current files of Reference Center holdings and JPCRD articles, including property and material terms, on the OSRD computer facility. This, in coordination with appropriate interfaces to the Bedford Composition System for computer typesetting, greatly facilitated the preparation of the latest publication list as well as the yearly indexes of the Journal. Other activities associated with the Reference Center have begun to be automated, with a tracking system for the review and production processes of publications in progress already in place on the HP.

#### Outside Interactions

OSRD continues to interact extensively with outside groups who wish to build and distribute on numeric databases, and staff members take initiative in leading these efforts. Examples of cooperative efforts include working with the Metal Properties Council, with DOE in building a Materials Database System, with AIChE on the DIPPR project, and with such international groups as CODATA and IUPAC. These activities continue to be very fruitful.

## DATA CENTER AND PROJECT REPORTS

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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.

## DATA CENTERS

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### ALLOY PHASE DIAGRAM DATA CENTER

J. G. Early, Director  
Institute for Materials Science and Engineering, 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, now a bimonthly publication, 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, as well as for input of data to the database.

A vigorous evaluation program for titanium systems, with support by ONR, has been completed, and more than 61 titanium binary systems have been evaluated. The completed compilation of evaluated titanium binary phase diagrams will be issued as an ASM Monograph. Evaluation of aluminum systems has continued, supported in part by DARPA, and more than 20 systems have been evaluated. In addition, work on iron systems supported in part by DOE is well underway, and three systems have been evaluated this year. During this evaluation effort, thermodynamic optimization program have been enhanced and interfaced with the graphics software.

The prototype user-friendly phase diagram database of graphical and numerical information is now complete. A new effort was initiated to digitize over 1500 binary phase diagrams for the new ASM compendium,

Constitution of Binary Alloys. As a result of this effort, a complete online database will be available with diagrams containing mutually consistent pure element properties and phase nomenclature. This is being done in close cooperation with the ASM. Currently, three ASM Research Associates are working in the Center.

### AQUEOUS ELECTROLYTE DATA CENTER

David Smith-Magowan, Director  
Center for Chemical Physics, NBS

The Center provides, to users in the scientific and industrial communities, critically evaluated data on the physical and chemical properties of aqueous electrolyte solutions, including activity coefficients, excess enthalpies, heat capacities and volumes, solubilities, EMF, viscosities, conductivities as well as others. It also provides techniques for the correlation and estimation of these properties and provides information/advise in response to requests by mail and telephone.

The technical activities of the Center are closely coordinated with the Chemical Thermodynamics Data Center, with both units participating in the maintenance and development of the bibliographic and abstract archives. These centers also share computer facilities.

The thermodynamic properties of calcium chloride solutions have been correlated as functions of temperature and composition as a test of the algorithm that is being developed to correlate properties with respect to temperature, composition and pressure. Values for excess Gibbs energies, enthalpies and heat capacities have been evaluated for concentrations from 0 to 11 molal between temperature of 298 and 373 K. Extension to higher temperatures and inclusion of pressure as an independent variable are underway.

Gibbs energies of formation for 30 substrates that are interconverted in the Krebs metabolic cycle (the principal energy producing pathway in aerobic organisms) have been evaluated by an analysis of the enzyme-catalyzed equilibria that comprise the cycle. This is the first study in over 25 years to integrate the equilibrium data for such an extensive network, and for many of the compounds studied, these are the first reference-quality values in aqueous solution to be evaluated.

#### 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 particle collisions. 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. An article on charge transfer of hydrogen atoms and ions in metal vapors was completed for the Journal of Physical and Chemical Reference Data. A review of proton-impact ionization of gaseous targets will appear in Reviews of Modern Physics. An evaluated compilation of collision strengths and cross sections for electron impact excitation of atomic ions was completed. This report will be particularly useful to the astrophysics community. JILA Fellow A. V. Phelps completed three reports which are tabulations of electron collision cross sections and calculated transport coefficients on  $N_2$ ,  $H_2$  and  $D_2$ , and  $O_2$ , respectively. Work continues on the review of measured cross sections for electron-impact excitation of atoms. Another major review in progress is "Collisional Alignment and Orientation of Atomic Outer Shells. I. Direct Excitation by Electron and Ion Impact."

Approximately 900 numerical data files have been entered into the Atomic Collisions Data Base. These are being used to prepare figures supporting the Center's review activities. Programs are being developed to produce listings and indices of the material in the Data Base and to provide an online enquiry capability.

## 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 in such areas as plasma diagnostics, laser physics and astronomy.

We have completed the most extensive compilation of data for magnetic-dipole (forbidden) spectral lines ever carried out. The data include more than 1400 wavelengths for atoms and ions of the elements beryllium through molybdenum ( $Z=4-42$ ) and also their calculated transition probabilities. The results are being submitted for publication in the Journal of Physical and Chemical Reference Data. Our compilation of energy levels for the 15 spectra of phosphorus was completed and is in press. We are now working on similar compilations for the sulfur and molybdenum spectra.

Work on the data for sulfur and molybdenum will continue. We plan to collaborate with physicists at the Japan Atomic Energy Research Institute on a publication of Grotrian diagrams for the molybdenum spectra. Pending availability of new data for some of the sulfur spectra, we will begin reviewing and compiling energy-level data for some of the chlorine spectra. As time permits, we will begin a database of (allowed) atomic spectral lines with compilations for certain spectra of molybdenum and/or iron-group elements.

## 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 radiative transition probabilities for atoms and atomic ions. These data are essential in such areas as plasma modelling and analysis, including fusion research, as well as laser physics and astrophysics.

The comprehensive compilation of atomic transition probability data for allowed lines in the elements scandium through nickel is nearly complete, and work is concentrating now on evaluating data on forbidden transitions in these elements. Critical reviews of Stark widths and shifts in neutral and ionized atomic species were published in JPCRD. A book "Spectroscopic Data for Iron" was assembled from existing NBS-NSRDS data compilations and was published as Volume IV of the new ORNL series "Atomic Data for Fusion" to serve the special data needs of the magnetic fusion community. A second book containing spectroscopic data for Ti and Ni ions is in preparation. A computerized database of bibliographic information on atomic energy levels, atomic transition probabilities, and atomic line shapes and shifts was designed; much of the implementation of input capability, as well as very limited retrieval and output capability, was completed in collaboration with the staff of OSRD.

Future plans call for completing the compilation of transition probabilities for scandium through nickel, at which point our work will shift to the light elements hydrogen through neon, as well as selected heavy elements (such as Kr and Zr). It is also planned to complete work on both input and output capability for the bibliographic database system. Input of references on atomic transition probabilities will be initiated. Long-range plans include the design and development of a computerized database of critically evaluated data on atomic spectroscopic quantities.

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.

The present OSRD project involves evaluated thermochemical data for alloys and elements.

#### CHEMICAL KINETICS DATA CENTER

J. T. Herron, Director  
Center for Chemical Physics, NBS

The Data Center is responsible for the compilation, evaluation and dissemination of data on the kinetics of elementary chemical reactions. The primary field of activity is gas phase reactions of neutral species. It maintains computer files on combustion related gas phase reaction rate data published since 1971, and provides critical evaluations of selected parts of that data base. It maintains files of archival publications and prepares critical evaluations in the area of stratospheric chemistry.

The compilation of experimental rate constants for combustion related reactions covering the period 1977 through 1982 is complete. Data have been abstracted for the year 1983, and articles identified for abstracting for the year 1984. The major evaluation activity on combustion chemistry has resulted in the publication of NBSIR84-2913 "Chemical Kinetic Data Base for Methane Combustion." This has been submitted to JPCRD for archival publication. It contains data on 235 reactions. Work has now been completed on an additional 164 reactions. In the area of stratospheric chemistry, the Data Center provides NASA with evaluated data on halogen reactions. The first part of a project on the chemistry of dielectric breakdown has been completed and manuscripts prepared on the subjects of the thermochemistry of S-F-0



compounds, and the kinetics of reactions of SF<sub>4</sub>, SF<sub>5</sub> and S<sub>2</sub>F<sub>10</sub>. Work also continues on the development of a computer based data management system for the storage, searching and accessing of chemical kinetic data.

In the coming year, the coverage of the Data Center will be expanded to include a broader range of gas phase reactions. All archival articles on the kinetics of gas phase reactions will be identified and added to the Data Center files. The range of abstracted data will be expanded accordingly. Evaluation of combustion data will continue with the inclusion of larger organic species. By the end of the year the total evaluated database will contain about 600 separate numerical entries. Work will continue on maintaining the halogen related stratospheric chemistry database. A joint activity between the Data Center and the Electrosystems Division of NBS will be continued with evaluation and estimation of rate parameters for the S-F-O reaction system. It is expected that the Data Base Management System for the Data Center will be complete this year.

#### 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. These critically evaluated data also are used in the design and interpretation of research in physics, chemistry, biochemistry, geochemistry, environmental science, metallurgy and other fields where chemical interactions are important. The Center provides data describing the change in the chemical properties of substances as well as bibliographic reference services on thermochemistry. In particular, the Center provides enthalpies and Gibbs energies of formation, entropies, C<sub>p</sub> in the standard state at 298.15 K and 1 bar, and enthalpies of formation at 0 K for inorganic substances and simple organic substances, and to a more limited extent transition properties, and thermal functions. The publication "The NBS Tables of Chemical Thermodynamic Properties" (1982) represents a major activity of the Center. It lists 26,000 data values pertinent to 14,000 substances. The experience gained in this work is now being applied in an international cooperative program under the auspices of CODATA.

The Center is cooperating with four others to design an ongoing system for evaluating thermodynamic data. Together they have produced a set of prototype tables. These tables, covering a number of compounds of calcium and some auxiliary substances, serve two purposes. One, they demonstrate the feasibility of producing chemical thermodynamic tables using decentralized highly-automated 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 provide a model for a new generation of tables. Toward the end of 1985 these tables will be made available for review and comment by the thermochemical community.

Each year the Center surveys the thermodynamic literature and extracts pertinent data. These go into its master index of thermodynamic measurement. This information is published annually as the Inorganic Section of the Bulletin of Chemical Thermodynamics.

The Center has made a major effort in the further development of data center techniques. The major purpose is full automation of the Center's data collection activities, for efficiency, flexibility and effective cooperation with other data projects. A standardized procedure has been established for entry of bibliographic data and for the extraction of data from experimental papers. Programs have also been implemented for processing of thermochemical data and thermal functions, as aids in the data evaluation process.

#### CORROSION DATA CENTER

G. M. Ugiansky, Director  
Institute for Materials Science and Engineering, NBS

The Corrosion Data Center is the NBS component of a joint program between the National Association of Corrosion Engineers (NACE) and NBS; it is concerned with the collection, evaluation, and effective dissemination of corrosion data. The central focus of the program is the establishment of an evaluated corrosion database which can be easily computer-accessed to provide the user with the required data in any of a number of possible graphical or tabular formats.

Several pilot projects have been initiated in the areas of kinetic and thermodynamic corrosion data. In the kinetic area, the projects include atmospheric corrosion of structural alloys, localized corrosion of stainless steel and other alloys, and uniform corrosion of alloys in aqueous and non-aqueous media. In the thermodynamic area, efforts have been focused on the use of computers for the calculation and display of stability diagrams of the electrochemical potential-pH type known as Pourbaix diagrams.

A major Workshop on Corrosion Data was held in June of this year, attended by over 50 corrosion specialists. High-priority data needs were identified which will be very important in setting the direction of future corrosion data evaluation projects.

During the coming year, the first databases will be released for personal computers. These databases will contain kinetic and thermodynamic data from traditional data sources and will provide the basis for future database activities.

#### CRYSTAL DATA CENTER

A. D. Mighell, Director  
Institute for Materials Science and Engineering, NBS

The Crystal Data Center is concerned with the collection, evaluation, and dissemination of data on solid state materials. The Center maintains a database which includes crystallographic and chemical information on all types of substances with known unit cells. The materials fall into the following categories: organics,

organometallics, metals, intermetallics, inorganics, and minerals. For each substance, the data include the cell parameters, the space group, compound name and formula, calculated density, critical comments, and literature reference. During the year, the database has been significantly upgraded and expanded. Approximately, 16,000 existing inorganic entries have been revised, processed by NBS\*AIDS83, evaluated, and added to the data base. In addition, - 5,000 organic entries corresponding to recently published data have been added.

To permit scientists to utilize the database, we are developing software tools that can be distributed with the database or used to search the database online at a central site. NBS search software, which became an integral part of the Crystal Data Distribution Package in June 1985 is designed to be used on a variety of computers. With the lattice-matching algorithm, unknown compounds can be identified by comparison with entries in the database once a cell has been determined using diffraction techniques. The lattice-matching method offers a comprehensive technique to characterize solid-state materials and is now in routine use at the National Bureau of Standards, in industrial analytical laboratories, and by crystallographic data centers.

An online search system is available through the Canadian Institute for Scientific and Technical Information and can be accessed online by any scientists in North America or Europe. The types of data that can be searched include chemical name and formula, cell parameters, cell volume, crystal system, space group symbol and number, density, bibliographic data, chemical class, plus additional data. During the year, this system has been used by the NBS Crystal Data Center and by individual scientists to solve a variety of scientific problems in diverse areas of chemistry and solid-state physics.

Immediate future efforts of the Data Center will focus on several areas of activity. First, the Data Center must become operational in our new computer environment. NBS\*AIDS83 will be adapted to the Hewlett Packard computer. Second, minerals data will be processed and evaluated in order to produce a book and a minerals subfile which can be marketed on a small computer such as the IBM PC computer. Third, the database and software components of the NBS Crystal Data Distribution Package will be enhanced. The NBS Crystal Data File will be expanded with respect to the number of entries and the data items per entry (e.g., a conventional cell will be added). The NBS\*LATTICE program will be expanded and the lattice-matching program function will be made more selective.

#### FLUID MIXTURES DATA CENTER

Neil A. 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 the mixtures -- mole fractions. A strong element in all of the work is the production of computerized data bases which are then disseminated by OSRD and other organizations.

A computer package called MIPROP has been completed which includes all of the fluids of "Thermophysical Properties of Fluids - I" and "Thermophysical Properties of Fluids - II." The package therefore calculates properties for hydrogen, nitrogen, oxygen, argon, ethylene, nitrogen trifluoride, methane, ethane, propane, isobutane, and normal butane. The package will be available from OSRD in the fall of 1985 in standard tape version and on microcomputer disk, which is designed to be compatible with most microcomputers.

A paper giving evaluated data for carbon monoxide equilibrium properties is complete and in press and a paper on the transport properties of argon is in IUPAC review.

A preliminary version of SUPERTRAPP is in the testing stages. When test and validation have been completed it will be made available on magnetic tape through OSRD. It will replace the current version of the TRAPP computer package.

Work is underway on the critical evaluation publications for the  $C_1 - C_4$  alkanes.

Future plans include theoretical studies leading to the development of new mixing rules, completion of SUPERTRAPP, critical evaluations of the properties of methanol and benzene, and completion of the corresponding states summary for methane-nitrogen system.

#### 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. It participates in the periodic development under the auspices of CODATA 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. The Center also publishes a quarterly preprint and reprint newsletter entitled "Preprints on Precision Measurement and Fundamental Constants" or PMFC; participates in the organization of conferences relating to the precision measurement-fundamental constants (PMFC) field; administers the NBS Precision Measurement Grant program; and participates in the work of various committees in the PMFC field.

The major activity of the Center during FY 85 involved working towards the completion of the 1985 least-squares adjustment of the constants. The set of best values resulting from this adjustment will replace the now nearly obsolete set resulting from the 1973 adjustment. The 1985 effort, like its 1973 predecessor, is being carried out by B. N. Taylor in collaboration with E. R. Cohen, Rockwell International, and under the sponsorship and guidance of the CODATA Task Group on Fundamental Constants (Dr. Cohen is current Task Group Chairman). As part of this effort, three papers on the fundamental physical constants were written and published: "Impact of Quantized Hall Resistance on SI Electrical Units and Fundamental Constants," *Metrologia* 21 37 (1985); "New Results from Previously Reported NBS Fundamental Constant Determinations," *J. Res. Natl. Bur. Stand.* 90, 91 (1985); and "Electrical Units, Fundamental Constants, and the 1983 Least-Squares Adjustment," *IEEE Trans. Instrum. Meas.* IM-34, 155 (1985).

The principal focus of the Center during FY 86 will be the completion and publication of the 1985 least-squares adjustment; it is expected that a CODATA Bulletin giving the new set of recommended values will be published in early 1986. Significant attention will also be given to the organization of one or more sessions on the fundamental constants and related work for the 1986 Conference on Precision Electromagnetic Measurements to be held at NBS-Gaithersburg, June 23-27, 1986.

#### ION KINETICS AND ENERGETICS DATA CENTER

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

Since the publication in 1969 of NSRDS-NBS 26, "Ionization Potentials, Appearance Potentials, and Heats of Formation of Gaseous Positive Ions," the Ion Kinetics and Energetics Data Center has been considered by the scientific public as the pre-eminent source of authoritative evaluated data on the thermochemistry of ions in the gas phase. The primary long range goals of the Data Center are to maintain up-to-date computer-searchable archives of data on ionization potentials appearance potentials, heats of formation of positive ions, ion-molecule reaction-rate constants and equilibrium constants, and to publish authoritative evaluations of those data.

Recent publications include: (1) "Evaluated Gas Phase Basicities and Proton Affinities of Molecules; Heats of Formation of Protonated Molecules" Sharon G. Lias, Joel F. Liebman, and Rhoda D. Levin, *Journal of Physical and Chemical Reference Data* 13, 695-808 (1984) (an up-date, including data from 28 relevant papers which appeared since the compilation went to press, was prepared and distributed with the reprints, more than 100 of which have been requested) and (2) "Absolute Values of Gas Phase Proton Affinities and Basicities of Molecules: A Comparison Between Theory and Experiment," D. A. Dixon and S. G. Lias, Molecular Structure and Energetics (J. F. Liebman and A. Greenberg, editors) VCH Publishers, Inc., Florida (in press), an evaluation of theoretical determinations of proton affinities which grew out of collaborative contacts between the Data Center and Dr. David A. Dixon of the E. I. DuPont de Nemours Company.

Currently in progress is the final work on "Ion Thermochemistry" by S. G. Lias, J. E. Bartmess, J. F. Liebman, J. L. Holmes, and R. D. Levin, a comprehensive and complete compilation of evaluated heats of formation of more than 3000 positive and negative ions, to be submitted soon for publication in the Journal of Physical and Chemical Reference Data. The evaluation of the data for the years before 1981 (covered in our 1982 unevaluated publication, R. D. Levin and S. G. Lias, "Ionization Potential and Appearance Potential Measurements, 1971-1981" and earlier Data Center publications) has been completed. Current work involves bringing the tables up-to-date by abstracting and evaluating all data which have appeared in the literature since 1981. The list of authors of this publication includes several outside collaborators, who bring specialized expertise to the project. These are Dr. J. E. Bartmess of the University of Tennessee (thermochemistry of anions), Dr. J. L. Holmes of the University of Ottawa (appearance potentials of ions, and derivation of thermochemical and structural information on ions from mass spectrometric data), and Dr. Joel F. Liebman of the University of Maryland Baltimore County (bonding theory and the estimation of thermochemical data).

Plans for an evaluated compilation of data on ion-molecule rate constants and reaction cross sections have been made and a literature search for that project has been initiated.

Dr. J. E. Bartmess of the University of Tennessee is maintaining computer-searchable up-to-date archives of anion thermochemistry as a continuing activity of the Data Center.

Extensive collaborative efforts on joint projects with the Chemical Kinetics, Chemical Thermodynamics, and Electrolyte Data Centers involving technical work on manuscript production, database design, documentation, and liaison efforts concerned with computer utilization were initiated during FY 85. Personnel from the Data Center are working in collaboration with the other data centers toward the documentation and implementation of a searchable database for the archival data on chemical kinetics as well as for ionization potential and appearance potential data.

#### 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.

A revised and updated comprehensive edition of the JANAF Tables will be published this year as a Supplement to the Journal of Physical and Chemical Reference Data.

The JANAF Center is one of the five centers involved in the preparation of the prototype CODATA Thermochemical Tables which are discussed in more detail under the Chemical Thermodynamic Data Center.

#### 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. Published reviews are designed to aid in the analysis and identification of compounds and to permit the determination of a wide range of molecular properties. One phase of the Center's work emphasizes microwave spectra of interstellar molecules.

Earlier this year a review of the microwave spectrum of  $\text{SO}_2$  was published in the Journal of Physical and Chemical Reference Data as part 22 of the series "Microwave Spectra of Molecules of Astrophysical Interest." A paper entitled, "Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions - 1984 Revision" has been accepted for publication in the Journal of Physical and Chemical Reference Data. This review provides the most accurate transition frequencies available for the 5 known interstellar species. It contains about 2545 transitions for 114 isotopic forms of these species.

During the next year we plan to complete a review on the microwave spectra of hydrocarbons as Part III of the series "Microwave Spectral Tables."

#### MOLTEN SALTS DATA CENTER

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

The Center compiles, evaluates and disseminates data on thermophysical properties of molten salt systems. Properties covered include density, electrical conductivity, viscosity, surface tension and selected thermodynamic properties including the eutectic points of mixtures.

Recommended values for properties of an extensive list of single and binary molten salt systems have been published in the Journal of Physical and Chemical Reference Data. At the present time, a concise updated summary publication in equation form is being prepared. At the same time, the data files of the Center are being automated. This automation will assist with the preparation and publication of the summary publication and simplify future updating.

Efforts are also underway to produce interactive automated products. A searchable comprehensive file of eutectic points has been completed. Other automated files to give numerical data for density, conductivity, viscosity and surface tension are being prepared. The data center is utilizing the Stanford SPIRES data base management system.

#### 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. Cook, Director  
Institute for Materials Science and Engineering, NBS

The Phase Diagrams for Ceramists Data Center is responsible for collecting and evaluating phase diagrams for inorganic, nonmetallic systems. More specifically, systems covered are: metal-oxygen systems, metal oxides, oxygen-containing radicals, halides, sulfides, and high-temperature ceramic systems containing gaseous components. Also covered are various combinations of these types of systems.

The goals of the Data Center are twofold: (1) maintenance of an up-to-date computerized database containing both bibliographic and graphic data and (2) provision of this information to the user community in readily accessible form, including timely publication of hardbound volumes. The Phase Diagrams for Ceramists Data Center works closely with the American Ceramic Society, which is responsible for the publication of "Phase Diagrams for Ceramists," a Data Center product.

During the current year, significant progress has been made in the computerization of the database. More than 5000 bibliographic entries have been keyboarded. A software package for efficient digitization, editing, and plotting of binary ceramic phase diagrams is now being used routinely. Many binary phase diagrams were plotted in camera-ready form



using this system. Work has progressed on a similar package for ternary systems, specifically designed for the most efficient use in this data center. Additionally, the task of evaluating diagrams for inclusion in Volumes 6 and 7 of the PDFC Series has progressed steadily.

During the next year, the momentum of the database computerization effort will be increased. Funds from the ACerS fundraising activity have become available so that ACerS research associates can be hired to work at NBS and assist with the task of database development. The utilization of thermochemical optimization and computer modeling methods in evaluation will be increased.

#### 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 as well as transport data pertaining to the penetration of radiation through bulk matter.

Activities during the past year include the following: (a) Through the synthesis of various theoretical approaches, a method has been developed for the accurate evaluation of the bremsstrahlung spectrum produced in Coulomb interactions between electrons and atoms. Extensive tabulations of these cross sections have been completed for all elements with atomic numbers  $Z = 1$  to 100, for electron energies between 1 keV and 10 GeV. The results have been published in two articles in technical journals, and a computer-readable tape of bremsstrahlung cross sections has also been prepared. (b) A predictive algorithm has been further developed which generates photon scattering, absorption, and pair-production cross sections, as well as attenuation coefficients, for any compound of specified composition. The algorithm involves use of the Center's database and the application of suitable interpolation procedures. The development has been pushed to the stage where the generation of photon cross sections can be easily carried out interactively from a computer terminal. (c) Preliminary tables have been prepared of proton stopping powers and ranges from about 200 materials in the energy region 1 keV to 1 GeV. These tables were generated using Bethe's stopping power theory above, and experimental data below, 1 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.

Critical reviews on superoxide rate constants in aqueous solution and on triplet-triplet absorption spectral data - representing more than 1143 individual organic species, will soon be published in JPCRD. Other data compilations in progress include: intersystem crossing quantum yields, one-electron reduction potentials involving radicals in aqueous solution, rate constants for transients in aqueous solutions of actinides, and rate constants for transients from water.

Several programs for automation of the Center are underway. These include programs to produce and prepare for publication tables of data indexes and reference lists. Programs for on-line searching of numerical data files are also being developed. A searchable on-line bibliographic data base is available to users of the Radiation Laboratory on DOE/RECON at Oak Ridge.

Publication of the biweekly and cumulative bibliographies is being continued.

#### THERMODYNAMIC RESEARCH CENTER

K. N. Marsh, Director  
Texas A&M University  
College Station, Texas

The Center provides 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 has been published in JPCRD. 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 paper has been accepted by the JPCRD. A third portion of the work involves the thermochemistry of these substances. Available enthalpies of reaction (primarily enthalpies of combustion) and equilibrium constants have been evaluated.

The Center also prepares the section on organic compounds for the Bulletin of Chemical Thermodynamics which 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.

Papers on the benzene-hexane and benzene-cyclohexane systems have been published and comprehensive papers on all other  $C_6 - C_6$  systems have been submitted for publication. Currently, work is being carried out on hydrocarbon-aliphatic alcohol systems.

## PROJECTS (Physical Data Program)

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### CRITICAL COMPILATION OF MASS SPECTRAL DATA

Steve Down  
Mass Spectral Data Centre  
Nottingham, England  
Source of Support: NBS

This project compiles, evaluates, and enters mass spectra into the Mass Spectral Database. The data are collected from the open literature and other sources, both public and private. Their quality is assessed through application of a quality index algorithm. The high-quality spectra are added to the database.

This year a new Memorandum of Understanding between NBS and the Royal Society of Chemistry has been drawn up. We are presently waiting for acceptance of that MOU by Nottingham. The new MOU is a direct result of the new management structure for the Mass Spectral Database Project. Upon acceptance of the MOU, NBS will resume support of mass spectral data collection and evaluation at Nottingham.

### COMPILATION OF ATOMIC WAVELENGTHS BELOW 2000 ANGSTROMS

Raymond L. Kelly  
U.S. Naval Postgraduate School  
Monterey, California  
Source of Support: NSF

This project has completed a compilation of atomic spectral lines with wavelengths below 2000 Å. A manuscript is being prepared for publication as a major supplement to the Journal of Physical and Chemical Reference Data. The compilation will cover the elements hydrogen through krypton.

In the future, this type of work will be done within the NBS Atomic Energy Levels Data Center. Increased NBS and OA resources have been obtained to allow the expansion in the Data Center.

### K SHELL IONIZATION BY HYDROGEN AND HELIUM IONS

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

This project has been completed, and a manuscript entitled "K Shell X-ray Production by Hydrogen and Helium Ions in The Elements (Z= 4 to 92)," has been submitted to the journal, Atomic and Nuclear Data Tables. The work presents x-ray production cross sections along with comparisons to theoretical results.

## DIGITIZATION OF THE COBLENTZ SOCIETY INFRARED DATABASE

William Strauss  
Johns Hopkins Applied Physics Laboratory  
Columbia, Maryland  
Source of Support: EPA, NIH

This project was established to digitize The Coblenz Society database of evaluated reference infrared spectra of substances in the condensed phase. A mini-computer-based digitization system at the Johns Hopkins Applied Physics Laboratory was utilized to generate the spectra.

The project has been completed. Magnetic tapes containing over 4100 digitized spectra have been delivered. Presently only the digitized spectra and substance identifier numbers are in automated form. Information such as substance names, formulas, etc., must be merged with the existing database.

## SOFT X-RAY INTERACTIONS WITH MATTER

E. B. Saloman  
National Bureau of Standards  
Gaithersburg, Maryland  
Source of Support: DOE, NBS

A pilot project is in progress within the Photon and Charged Particle Data Center to compile and evaluate soft x-ray cross sections (100 eV to 10 keV). Requirements for these cross sections exist, for example, in the following fields: lithography in the manufacture of integrated circuits, EXAFS method for determination of atomic distributions in amorphous materials, trace element analysis by x-ray emission spectroscopy, nuclear explosion diagnostics, design of x-ray lasers, and calculation of x-ray and particle beam radiation effects.

A study has been carried out in the energy region 1-100 keV of the total experimental database of x-ray cross sections versus the theoretical results using Scofield's photoionization cross sections for elements  $Z=1-92$ . Another study is in progress covering the energy range 100-1000 eV, comparing the experimental database for elements  $Z=1-92$  with Henke's semi-empirical data and Scofield's theoretical calculation (both direct and renormalized). The preliminary results indicate that for this energy range it is better not to perform Hartree-Slater to Hartree-Fock renormalization on the theoretical calculation. The graphical results show directly the status of agreement between theory, Henke's recommendations, and the various data sets. They permit the user to evaluate the uncertainty of a given choice of cross section value.

## MEDICAL PHYSICS DATA BOOK (2ND edition)

Medical Physics Data Group  
American Association of Physicists in Medicine  
Source of Support: AAPM, NBS

The American Association of Physicists in Medicine (AAPM) has requested that a second edition of the highly successful Medical Physics Data Book be produced for use by hospital physicists. The handbook, which provides physical and chemical data related to radiologic and nuclear diagnostic and therapeutic techniques, will be expanded to include new information in all existing areas as well as subjects such as nuclear magnetic resonance (NMR) imaging.

Work is being carried out by the Medical Physics Data Group of the AAPM. This group was constituted by the Association to monitor important data requirements and respond to them.

## CRITICAL COMPILATIONS AND REVIEWS OF DATA DESCRIBING THE ELECTRON IMPACT EXCITATION OF ATOMS AND ATOMIC IONS

Jean W. Gallagher  
University of Colorado  
Boulder, Colorado  
Source of Support: NSF

This project will support three related efforts which all address aspects of the fundamental process of electron impact excitation of atoms and singly- and multiply-charged atomic ions. 1) Measured cross sections and excitation functions will be reviewed. 2) Collisional alignment and orientation of the charge cloud will be reviewed and compared to theoretical data. 3) Calculated collision strengths and cross sections for all atomic ions and transitions reported in the last two decades will be evaluated, and the most accurate data will be compiled.

## SPECTROSCOPIC PROPERTIES OF EXCITED ELECTRONIC STATES OF SMALL POLYATOMIC TRANSIENT MOLECULES

Marilyn E. Jacox  
National Bureau of Standards  
Gaithersburg, Maryland  
Source of Support: DOE

This project will prepare a compilation of experimentally determined spectroscopic properties of the bound and dissociative excited electronic states of covalently bonded transient molecules. This compilation will be useful to spectroscopists, photochemists, laser scientists, quantum chemists, chemical kineticists, and surface scientists concerned with problems in such diverse fields as combustion, energy generation, atmospheric chemistry, and chemical synthesis.

## PROJECTS (Chemical Data Program)

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### DATA ON AQUEOUS ELECTROLYTES

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

This project is closely coordinated with the work of the Aqueous Electrolyte Data Center. It is concerned with the evaluation, correlation, and prediction of data on the thermodynamic properties of aqueous electrolyte solutions. Methods for the computerized transfer of data files are also being investigated.

A primary objective is the development of methods for expressing the thermodynamic properties of aqueous electrolyte solutions over a wide range of temperatures. This year, a new correlation was developed for the thermodynamic properties of  $\text{CaCl}_2$  solutions.

In addition, a protocol for the computer transfer of electrolyte solution properties data is now being tested.

### PROPERTIES OF TRANSITION METAL COORDINATION COMPLEXES

M. Z. Hoffman  
Boston University  
Boston, Massachusetts  
Source of Support: DOE

This project is developing four data compilations related to transition metal coordination complexes. Specifically, the four compilations will be: 1) Optical absorption spectra of excited states, coordinated radical species, and systems in unusual oxidation states; 2) Photophysical and photochemical parameters; 3) Rate constants of excited state electron transfer reactions; and 4) Rate constants of excited state energy transfer reactions.

The format of the tables is now well established, as are the criteria for critical evaluation. Effort is being placed during the next quarter on entering Ru data. This should bring Ru data to approximately 67% completion; some other elemental groups are now at the 80-90% level.

## 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 behavior in the critical regions.

In September 1984, the International Association for the Properties of Steam adopted the formulations of the thermodynamic properties of H<sub>2</sub>O and D<sub>2</sub>O and authorized the preparation of the releases. These were written and circulated among all member countries by the end of 1984. After receiving input from some member countries, these releases were finalized.

During the past year, a draft release was also prepared for the thermal conductivity and viscosity of H<sub>2</sub>O. This release was adopted, subject to editorial changes, at the IAPS executive meeting in September, 1985.

## PROPERTIES OF POLAR FLUIDS

L. Haar, J. M. H. Levelt Sengers, and J. S. Gallagher  
National Bureau of Standards  
Gaithersburg, Maryland  
Source of Support: NBS

The polar fluids project has turned toward the development of a thermodynamic surface for the mixture of H<sub>2</sub>O and CO<sub>2</sub>. The methods being utilized are based on the theoretical techniques developed for the thermodynamic surface of H<sub>2</sub>O.

The ability to calculate the surface for a mixture is dependent on accurately describing the interactions between unlike molecules. It is hoped that further development of these procedures will lead to the ability to determine the thermodynamic surface for mixtures of polar molecules.



## CHEMICAL THERMODYNAMIC PROPERTIES OF POLYCYCLIC AROMATIC HYDROCARBONS

R. Alberty  
Massachusetts Institute of Technology  
Cambridge, Massachusetts  
Source of Support: DOE

Tables of standard chemical thermodynamic properties of polycyclic aromatic hydrocarbons are being calculated from the best available data and extended to higher temperatures and higher carbon numbers by use of the Benson method. These tables for the ideal gas phase are to cover 298 K to 3000 K because of the importance of these data in understanding soot formation in flames and the high temperature vaporization of graphite.

Articles will be prepared for the Journal of Physical and Chemical Reference Data giving in addition, reviews of the databases and an assessment of the accuracy of the calculated values.

## BINARY VAPOR-LIQUID EQUILIBRIUM DATA FOR LIGHT HYDROCARBONS WITH METHANE

K. E. Starling  
University of Oklahoma  
Norman, Oklahoma  
Source of Support: DOE

This project will develop a critical compilation of binary vapor-liquid equilibrium (VLE) data for light hydrocarbons with methane. A literature survey of available VLE data for binary mixtures of methane with hydrocarbons up to n-decane will be conducted. Thermodynamic consistency tests will be performed to detect erroneous data.

## 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.

An additional 217 data sheets are being prepared. Systems covered are:

$H_2-O_2$ , hydrocarbon- $O_2$ , hydrogen-halogen, metal- $O_2$ ,  
 $O_2$  energy transfer, haloalkane- $O_2$ ,  $NH_3-O_2$ .

## DIPPR DATA PROJECTS

AIChE

New York, New York

Source of Support: NBS, Industry

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

NBS is involved with 3 DIPPR activities: the preparation of a data prediction manual, preparation of a data book on phase equilibria in aqueous electrolyte systems and a data compilation for industrially important chemicals. NBS supports the preparation of the data prediction manual and also the preparation of an automated version of the manual. The data book on aqueous electrolytes is being readied for publication. It will contain data and bibliographies prepared by NBS.

NBS also supported the preparation of an interactive automated version of the data compilation which will, when completed, provide access to data on over 1,000 selected compounds. The first version of that database is nearly complete. NBS and AIChE have also signed a new agreement which outlines how the two organizations will cooperate in disseminating the DIPPR database.

## 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 have recently been published.

These techniques are now being applied to a somewhat more complex set of fluids:  $H_2$ ,  $N_2$ ,  $O_2$ ,  $CO$ ,  $CO_2$ ,  $N_2O$ ,  $CH_4$ ,  $C_2H_4$ ,  $C_2H_6$ ,  $CF_6$  and  $SF_6$ . 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. These methods will also be extended to include some polar gases such as the weakly polar  $NO$  and the more strongly polar  $HCl$ ,  $H_2$ , and  $SO_2$ .

INTERNATIONAL CENTER FOR THE SYSTEMATIC CORRELATION AND  
DISSEMINATION OF THE TRANSPORT PROPERTIES OF FLUIDS

J. Kestin  
Brown University  
Providence, Rhode Island  
Source of Support: NBS

This project supports the Center for the Systematic Correlation and Dissemination of the Transport Properties of Fluids. The Center was established to coordinate the work of the groups associated with the Subcommittee on Transport Properties of Commission I.2 (thermodynamics) of the International Union of Pure and Applied Chemistry (IUPAC).

The Subcommittee concerns itself with topics of international scientific or technical significance requiring agreement, regulations, standardization, or codification in some aspect of pure or applied chemistry. Present activities fall into three projects: 1) Definitive correlation of the transport properties of gases with emphasis on data for the chemical industry; 2) Creation of an internationally available data bank of recently published or still unpublished experimental data on transport properties; and 3) Formulations of standards of viscosity and thermal conductivity in cooperation with the standards institutions of Japan, the United States, and the Federal Republic of Germany.

## PROJECTS (Materials Properties)

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### 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 numerical crystallographic data and references for organic and organometallic materials. From these entries, selected information will be used to update the NBS Crystal Data ID File, which is available for on-line use.

### OSRD BINARY PHASE DIAGRAM EVALUATION PROJECTS

#### Rare Earth Alloys

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

#### Copper Alloys

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

## VANADIUM AND NIOBIUM ALLOYS

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

## TITANIUM ALLOYS

J. Murray  
National Bureau of Standards  
Gaithersburg, Maryland  
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: NSF

## ACTINIDE ALLOYS

D. Peterson  
Los Alamos National Laboratory  
Los Alamos, New Mexico  
Source of Support: DOE

These evaluation projects are a major part the National Bureau of Standards-American Society for 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.

## PROPERTIES OF GLASSY-FORMING MELTS

L. D. Pye  
Alfred University  
Alfred, New York  
Source of Support: NSF

As part of a cooperative data program of the International Commission on Glass, the project will critically examine physical and thermodynamic properties of glassy-forming melts. The resulting compilation will replace existing out-of-date work and will enable the development of further high-tech uses of glass in extreme and unusual service conditions.

## SURFACE STRUCTURES DETERMINED BY LEED CRYSTALLOGRAPHY

P. R. Watson  
Oregon State University  
Corvallis, Oregon  
Source of Support: NSF

The primary technique for determining the geometrical arrangement of atoms in a surface or in an adsorbed layer is low-energy electron diffraction (LEED). Because experimental LEED cannot be directly inverted to yield unique data, iterative fit procedures are used. This project will critically examine all LEED and assess their quality. It will cover elemental surfaces and the compound ionics and semiconductors. Structures formed by adsorption will also be included.

## CREVICE CORROSION BEHAVIOR OF STAINLESS STEELS IN MARINE ENVIRONMENTS

T. S. Lee  
LaQue Center for Corrosion Technology  
Wrightsville Beach, North Carolina  
Source of Support: NSF

Stainless steels are widely used in marine construction as materials for heat exchangers, condensers, piping, and other applications. For service below 50 °C, material selection in these environments is generally based on its relative resistance to crevice corrosion. At present, data exist from service experience and laboratory tests.

This extensive database will be critically analyzed and summarized. The result will be a critical compilation of conditions under which a given material can be expected to undergo crevice corrosion and the rate of that corrosion. A wide range of stainless steels and service conditions will be included.

## COMPUTER EVALUATION MODELS FOR POWDER DIFFRACTION DATA

E. Evans and W. Wong-Ng  
JCPDS-International Centre for Diffraction Data  
Swarthmore, Pennsylvania  
Source of Support: NSF

Powder diffraction analysis is perhaps the technique most widely used to identify solid materials. In recent years, new computer methods for evaluating these data have been developed and applied to the powder data collection, identifying many problems. This project will examine all problem powder data to resolve the problems. In addition, a model will be developed for comparing calculated and experimental powder patterns.

## THERMOCHEMICAL MODELING OF COMPLEX CERAMIC PHASE EQUILIBRIA

K. E. Spear  
Pennsylvania State University  
University Park, Pennsylvania  
Source of Support: DOE

This project will develop and test a thermodynamic solution model and database for representing complex equilibria in multicomponent liquid oxide systems of industrial importance. In particular, the model will be used to calculate higher-order system phase equilibria. Such a model would greatly facilitate extending ceramic phase diagrams into regions where no experimental data exist.

## DUCTILE FRACTURE TOUGHNESS OF HIGH-STRENGTH LOW-ALLOY STEELS

F. Ebrahimi  
University of Florida  
Gainesville, Florida  
Source of Support: DOE

Although structural codes and specifications are more frequently based on fracture mechanics principles, the toughness tests specified for materials selection and quality control involve simple tests, such as the Charpy V-Notch Test. The fracture toughness value for ductile crack initiation has been advanced as the parameter that comes nearest to being a material property.

In this study, the ductile fracture toughness data for high-strength low-alloy steels will be critically reviewed on the basis of testing method, specimen geometry, and data reduction techniques. The results will include tensile properties if available.

## POLYMER SOLUTION MOLECULAR WEIGHT AND VISCOSITY PROJECT

H. Wagner  
National Bureau of Standards  
Gaithersburg, Maryland  
Source of Support: NBS

Many properties of high polymers are dependent on their molecular weight, so its proper measurement is essential for control and specification. A variety of methods have been developed to measure the molecular weight. One of the most valuable is that based on viscosity--an empirical relationship known as the Marck-Houwink equation. This project evaluates the empirically-determined constants used for linear polyethylene in five commonly used solvents as well as a number of theta solvents.

## 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  
Knowledge Systems, Inc.  
Scotia, New York  
Source of Support: Army

The move towards providing computer access to materials data such as mechanical properties has led to some potential problems 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.



## SURFACE SPUTTERING YIELD PROJECT

Joseph Fine  
National Bureau of Standards  
Gaithersburg, Maryland  
Source of Support: DOE and NBS

Sputtering techniques for depth profile are used in a number of methods to analyze compositional changes of materials at surfaces and interfaces. Many of these techniques have matured to being able to provide quantitative sputter depth profile information, yet the necessary data are not readily available in easy-to-use, evaluated form. This project will prepare a compilation of evaluated sputtering yield data for several ion species and energies for targets of pure elements.

## 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.

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Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range  $C_1$  to  $C_4$ . Part 1. Properties of Condensed Phases  
Randolph C. Wilhoit, Jing Chao, and Kenneth R. Hall

Standard Chemical Thermodynamic Properties of Alkylbenzene Isomer Groups  
Robert A. Alberty

Assessment of Critical Parameter Values for  $H_2O$  and  $D_2O$   
J. M. H. Levelt Sengers, J. Straub, K. Watanabe, and P. G. Hill

The Viscosity of Nitrogen, Oxygen, and Their Binary Mixtures in the Limit of Zero Density  
Wendy A. Cole and William A. Wakeham

The Thermal Conductivity of Fluid Air  
K. Stephan and A. Laesecke

The Electronic Spectrum and Energy Levels of the Deuterium Molecule  
Robert S. Freund, James A. Schiavone, and H. M. Crosswhite

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Microwave Spectra of Molecules of Astrophysical Interest. XXII.  
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Evaluation of the Thermodynamic Functions for Aqueous Sodium Chloride from Equilibrium and Calorimetric Measurements below  $154^\circ C$   
E. Colin W. Clarke and David N. Glew

The Mark-Houwink-Sakurada Equation for the Viscosity of Linear Polyethylene  
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The Solubility of Mercury and Some Sparingly Soluble Mercury Salts in Water and Aqueous Electrolyte Solutions  
H. Lawrence Clever, Susan A. Johnson, and M. Elizabeth Derrick

A Review and Evaluation of the Phase Equilibria, Liquid-Phase Heats of Mixing and Excess Volumes, and Gas-Phase PVT Measurements for Nitrogen + Methane  
A. J. Kidnay, R. C. Miller, E. D. Sloan, and M. J. Hiza

The Homogeneous Nucleation Limits of Liquids  
C. T. Avedisian

Binding Energies in Atomic Negative Ions: II  
H. Hotop and W. C. Lineberger

Energy Levels of Phosphorus, PI through PXV  
W. C. Martin, Romuald Zalubas, and Arlene Musgrove

Standard Chemical Thermodynamic Properties of Alkene Isomer Groups  
Robert A. Alberty and Catherine A. Gehrig

Standard Chemical Thermodynamic Properties of Alkylnaphthalene Isomer  
Groups  
Robert A. Alberty and Theodore M. Bloomstein

No. 4

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

Refractive Index of Water and Its Dependence on Wavelength, Temperature,  
and Density  
I. Thormahlen, J. Straub, and U. Grigull

Viscosity and Thermal Conductivity of Dry Air in the Gaseous Phase  
K. Kadoya, N. Matsunaga, and A. Nagashima

Charge Transfer of Hydrogen Ions and Atoms in Metal Vapors  
T. J. Morgan, R. E. Olson, A. S. Schlachter, and J. W. Gallagher

Reactivity of HO<sub>2</sub>/O<sub>2</sub> Radicals in Aqueous Solution  
Benon H. J. Bielski, Diane E. Cabelli, Ravindra L. Arudi, and  
Alberta B. Ross

The Mark-Houwink-Sakurada Equation for the Viscosity of Atactic  
Polystyrene  
Herman L. Wagner

Standard Chemical Thermodynamic Properties of Alkylcyclopentane Isomer  
Groups, Alkylcyclohexane Isomer Groups, and Combined Isomer Groups  
Robert A. Alberty and Young S. Ha

## Supplements

JANAF Thermochemical Tables, third edition

M. W. Chase, Jr., C. A. Davies, J. R. Downey, Jr., D. J. Frurip,  
R. A. McDonald, and A. N. Syverud  
(Supplement 1)

Atomic Energy Levels of the Iron Period Elements: Potassium through  
Nickel,

J. Sugar and C. Corliss  
(Supplement 2)

## Data Publications in NBS Series

Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet  
Table - O III

Charlotte E. Moore  
NSRDS-NBS 3, Section 11

## Other Publications in NBS Series

PIPE/1000 - An Implementation of Piping on an HP-1000 minicomputer

N.L. Seidenman  
NBS Technical Note 1208

Chemical Thermodynamics in Steam Power Cycles: Data Requirements

Otakar Jonas and Howard J. White, Jr.  
NBSIR 85-3205

Computerizing Materials Data - A Workshop for the Nuclear Power Industry

John Rumble, Jr., and Jack H. Westbrook  
NBS-SP 689

Standards and Metadata Requirements for Computerization of Selected  
Mechanical Properties of Metallic Materials

Jack H. Westbrook  
NBS-SP 702

Standard Reference Data Publications - 1964-1984

Joan C. Sauerwein and Geraldine R. Dalton  
NBS-SP 708

## Data Publications from Other Publishers

Bulletin of Alloy Phase Diagrams, Vols. 5 & 6, 1985

L. H. Bennett, Editor  
American Society for Metals  
(Evaluations done by NBS Alloy Phase Diagram Data Center and  
OSRD-funded projects)

Ag-Dy  
Ag-Er  
Ag-Eu  
Ag-Nd  
Ag-Pr  
Ag-Gd

Ba-Li  
Ba-Rb  
Ba-Cr  
Be-Cs  
Be-K  
Be-Li

Fe-Mg  
Fe-Au  
Fe-Rh  
Ga-Ti  
In-V  
K-Mg

Ag-Ho	Be-Na	K-Sr
Ag-Sm	Be-Rb	Mg-Rb
Ag-Tb	Bi-Ti	Mg-Na
Ag-Tm	C-V	Na-Sr
Ag-Yb	Ca-Cr	Np-Pu
Ag-Fe	Ca-Cs	Np-U
Al-Sb	Ca-K	Pb-Ti
Al-Hg	Ca-Na	Pu-Th
Al-P	Ca-Rb	Rb-Sr
Al-As	Ca-Cu	Si-V
Ba-K	Cr-Mg	Th-V
Ba-Na	Cr-Rd	
Ba-Cu	Cr-Sr	
Ba-Cs	Cu-Pb	

### Bibliographies and Indexes from Other Publishers

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Vol. 18, 1985

Radiation Chemistry Data Center

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Vol. 17, 1984

Radiation Chemistry Data Center

Bulletin of Chemical Thermodynamics, Vol. 26, 1983

Robert D. Freeman, editor

IUPAC Commission on Thermodynamics and Thermochemistry

Journal of Physical and Chemical Reference Data

Triplet-Triplet Absorption Spectra of Organic Molecules in Condensed Phases

Ian Carmichael and Gordon Hug

Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions-1984 Revision

F. J. Lovas

Thermodynamic Properties of Ethylene from the Freezing Line to 450 K at Pressures to 260 MPa

M. Jahangiri, R. T. Jacobsen, and R. B. Stewart

Standard Chemical Thermodynamic Properties of Alkyne Isomer Groups

Robert A. Alberty and Ellen Burmenko

New International Formulations for the Thermodynamic Properties of Light and Heavy Water

J. Kestin and J. V. Sengers

Thermodynamic Properties of Twenty-One Monocyclic Hydrocarbons

O. V. Dorofeeva, L. V. Gurvich, and V. S. Jorish

Thermodynamic Properties of Iron and Silicon

P. D. Desai

Electrical Resistivity of Chromium, Cobalt, Iron and Nickel

T. K. Chu and C. Y. Ho

High Temperature Vaporization Behavior of Oxides

R. H. Lamoreaux and D. L. Hildenbrand

Thermochemical Data on Gas-Phase Ion-Molecule Association and Clustering Reactions

R. G. Keese and A. W. Castleman, Jr.

Electrical Resistivity of Niobium and Titanium

R. N. Bogaard, H. M. James, and C. Y. Ho

Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C1 to C4 Part 2 Ideal Gas Properties

Jing Chao, Kenneth R. Hall, and Kenneth N. Marsh

Computer Methods Applied to the Assessment of Thermodynamic Data

S. P. Kirby, E. M. Marshall, and J. B. Pedley

Evaluated Kinetic Data for High Temperature Reactions Volume 5  
D. L. Baulch, M. Bowers, and D. G. Malcolm

Thermodynamic Properties of Selected Elements  
P. D. Desai

Thermodynamic Properties of Nitrogen from the Freezing Line to 2000K at  
Pressures to 1000 MPa  
R. T. Jacobsen, R. B. Stewart, and M. Jahangiri

Cross-Sections for Collisions of Electrons and Photons with Nitrogen  
Molecules  
Y. Itikawa, M. Hayashi and A. Ichimura

Thermodynamic Properties of Selected Binary Aluminum Alloy Systems  
P. D. Desai

Chemical Kinetic Data Base for Methane Combustion  
W. Tsang and R. L. Hampson

#### Supplements

Atomic and Ionic Spectrum Lines Below 2000 Angstroms  
Raymond L. Kelly

#### NSRDS-NBS Series Publications Scheduled for 1986

Tables of Experimental Rate Constants for Chemical Reactions Occurring in  
Combustion (1971-1982)  
J. Herron

#### Data Publications from Other Publishers Scheduled in 1986

Medical Linear Accelerator Central Axis Depth-Dose Data  
J. A. Purdy, W. B. Harms, and S. P. Fivozinsky

NBS/EPA/NIH/MSDC Mass Spectral Database  
W. Budde and S. P. Fivozinsky

#### Bibliographies and Indexed from Other Publishers Scheduled in 1986

Biweekly List of Papers on Radiation Chemistry and Photochemistry,  
Vol. 19, 1986  
Radiation Chemistry Data Center

Biweekly List of Papers on Radiation Chemistry and Photochemistry,  
Annual Cumulation with Keyword and Author Indexes, Vol. 18, 1985  
Radiation Chemistry Data Center

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





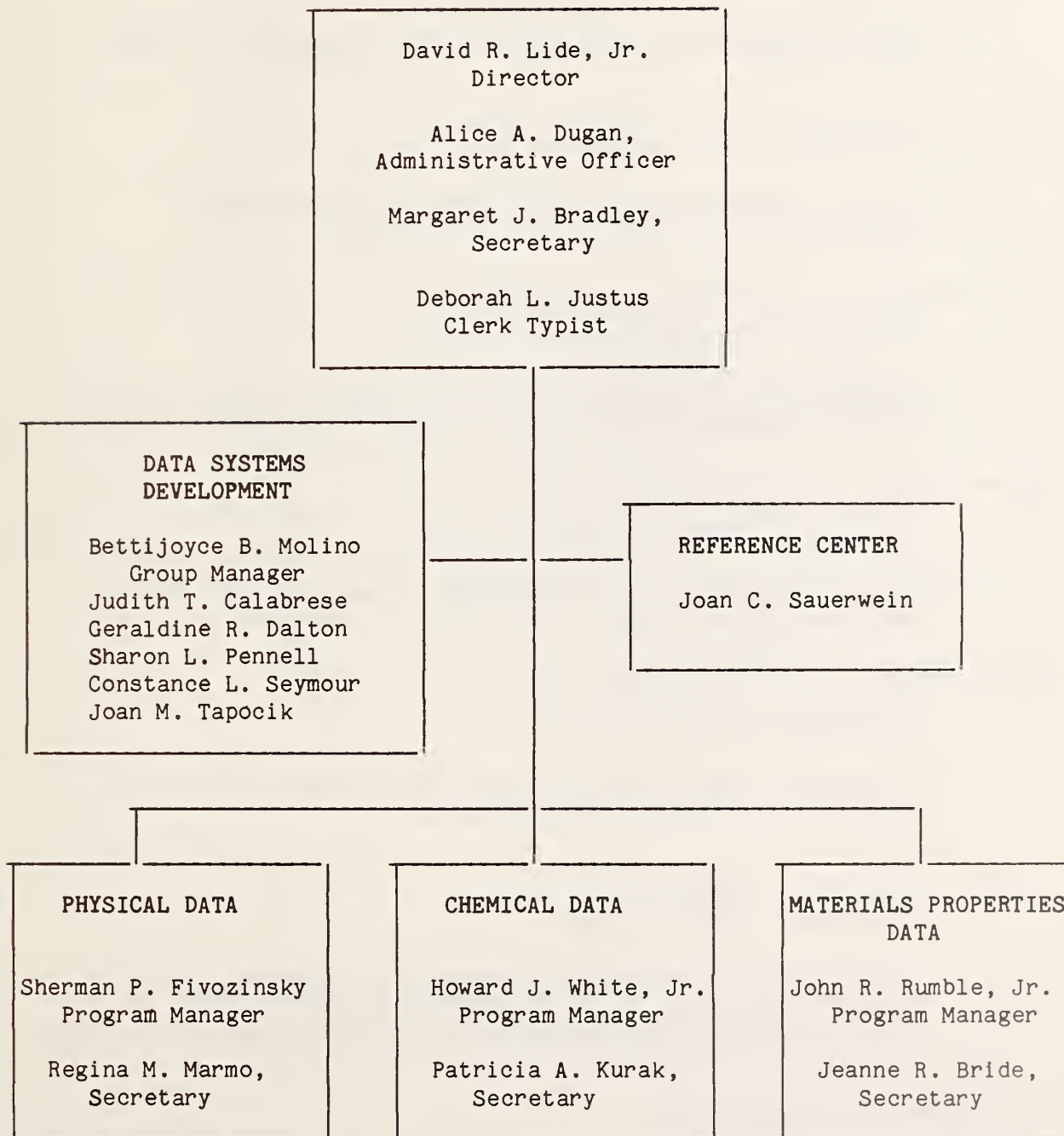
## LIST OF ACRONYMS AND ABBREVIATIONS

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AAAS	American Association for the Advancement of Science
AAPM	American Association of Physicists in Medicine (AIP)
ACerS	American Ceramic Society
ACS	American Chemical Society
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
APL	Johns Hopkins Applied Physics Laboratory
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
CAC	Center for Analytical Chemistry, NML, NBS
CAD	Computer-Aided Design
CAM	Computer-Aided Manufacturing
CAS	Chemical Abstracts Service
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
CISTI	Canada Institute for Scientific and Technical Information
CODATA	Committee on Data for Science and Technology (ICSU)
CRR	Center for Radiation Research, NML, NBS
CSIN	Chemical Substances Information Network
DARCOM	Department of The Army Command
DARPA	Defense Advanced Research Projects Agency
DECHEMA	Deutsche Gesellschaft für chemisches Apparatewesen
DIPPR	Design Institute for Physical Property Data (AIChE)
DOD	U. S. Department of Defense
DOE	U. S. Department of Energy
EMF	Electro-Motive Force
EPA	U. S. Environmental Protection Agency
ESCA	Electron Spectroscopy for Chemical Analysis
EXAFS	Extended X-ray Absorption Fine Structure
FDA	Food and Drug Administration
FIZ	Fachinformationszentrum
FY	Fiscal Year
GPE	General Purpose Equipment
GPSDC	General Purpose Scientific Document Code
GRI	Gas Research Institute
HP	Hewlett-Packard
IAPS	International Association for the Properties of Steam
ICDD	International Centre for Diffraction Data (JCPDS)
ICSU	International Council of Scientific Unions
IMSE	Institute for Materials Science and Engineering

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-University of Colorado
LEED	Low Energy Electron Diffraction
MPC	Metal Properties Council
MSDC	Mass Spectral Data Centre (UK)
NACE	National Association of Corrosion Engineers
NAS	National Academy of Sciences
NBS	National Bureau of Standards
NCI	National Cancer Institute
NEL	National Engineering Laboratory, NBS
NIH	National Institutes of Health
NLM	National Library of Medicine
NML	National Measurement Laboratory, NBS
NMPDN	National Materials Property Data Network
NMR	Nuclear Magnetic Resonance
NRC	National Research Council
NSF	National Science Foundation
NSRDS	National Standard Reference Data System
OA	Other Agency (Funding)
OMS	Office of Measurement Services, NML, NBS
ONR	Office of Naval Research
OSRD	Office of Standard Reference Data, NML, NBS
OSTP	Office of Science and Technology Policy
PDFC	Phase Diagrams for Ceramists Data Center
PL	Public law
PMFC	Precision Measurements - Fundamental Constants
PMS	Physical Measurement Services
RCDC	Radiation Chemistry Data Center
SAE	Society of Automotive Engineers
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

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Maintenance and enhancement of OSRD's Hewlett Packard 1000; user interface to HP 1000, programming support

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General programming support; development of microcomputer versions of databases and software

PUBLICATIONS BY OSRD STAFF

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Tools for the Automated Handling of Evaluated Data, Bettijoyce B. Molino, Proceedings of the 9th International CODATA Conference (North-Holland Publishing Company, 1985)

The Role of Computers in the Generation and Dissemination of Technical Data, David R. Lide, Jr., 10th IAPS Conference Proceedings

Chemical and Spectral Databases: A Look into the Future, John R. Rumble, Jr. and David R. Lide, Jr., J. Chem. Info. Comp. Sci. 25, 231-235 (1985)

Computerizing Materials Data - A Workshop for the Nuclear Power Industry, John Rumble, Jr. and Jack H. Westbrook, NBS Special Publication 689 (U.S. Department of Commerce, Washington, DC, 1985)

Computerized Materials Data - A Workshop for Ground Vehicle Engineering, John Rumble, Jr., M. R. Mitchell, and R. Thomas Northrup (Society of Automotive Engineers, Inc., Warrendale, PA, 1985)

Chemical Thermodynamics in Steam Power Cycles Data Requirements, Proceedings of a Workshop held at the National Bureau of Standards, Gaithersburg, Maryland, February 8-9, 1983, Howard J. White, Jr., Otakar Jonas, NBSIR 85-3205.

Thermodynamic Data Bases in the U.S. National Standard Reference Data System, Howard J. White, Jr., Proceedings of The First CODATA Symposium on Chemical Thermodynamic and Thermophysical Properties Data Bases, Paris, France, September 9-10, 1985,

INVITED TALKS AND PRESENTATIONS BY OSRD STAFF

---

Introduction to Bedford Mark-up, NBS, Gaithersburg, MD, April 1985  
Judith T. Calabrese

Workshop on Bedford Mark-up, NBS, Gaithersburg, MD, April 1985  
Judith T. Calabrese

Automated Production of Bibliographic Files Using the ABCUP Programs,  
NBS, Gaithersburg, MD, May 1985  
Geraldine Dalton

A Report on the Infrared Spectra Digitization Project Joint Committee on  
Atomic and Molecular Physical Data Meeting, New Orleans LA, Feb 1985.  
Sherman P. Fivozinsky

The NBS Standard Reference Data Program, DOC Productivity Theme Task Group  
on Information, Washington, DC, February, 1985.  
Sherman P. Fivozinsky

The OSRD Physical Data Program (round table participant) Workshop on  
Atomic Data for Fusion and Astrophysics, Daresbury Laboratory, Warrington,  
England, March 1985  
Sherman P. Fivozinsky

New Computer-readable Databases of Electron and Positron Stopping Powers  
and Photon Interaction Cross Sections, AAPM Annual Meeting Seattle,  
Washington, August, 1985.  
Sherman P. Fivozinsky

National and International Reference Data Programs, Bell Laboratories,  
Muray Hill, NJ, April 10, 1985  
David R. Lide, Jr.

The Role of CODATA in Database Development. First CODATA Symposium on  
Thermodynamic and Thermophysical Property Database, Paris, September 10,  
1985.  
David R. Lide, Jr.

Support for Critical Data Compilations in the United States, ACS Committee  
on Science, Task Force on Scientific Numerical Data Meeting, Miami Beach,  
FL, May, 1985.  
David R. Lide, Jr.

Overview of HP 1000 Upgrade from F-Series to A-Series for All Users,  
NBS, Gaithersburg, MD, February 1985  
Sharon Pennell

Computerized Materials Data, January 1985  
Symposium on Information Science, Science Council of Japan, Tokyo  
Department of Nuclear Engineering, Tokyo University  
Ministry of International Trade and Industry, Tokyo  
Institute of Information Science and Electronics, University of Tsukuba  
National Research Institute of Metrology, Tsukuba  
John R. Rumble, Jr.

Progress Towards Computer Access to Materials Data, WATtec National Energy Conference, Knoxville, TN, February 1985

John R. Rumble, Jr.

Computerized Materials Data, Annual Meeting of Gasket Fabrication Association, St. Petersburg, FL, March 1985

John R. Rumble, Jr.

Chemical Bonding Models - How Electron Scattering Tests Them, Tulane University, New Orleans, LA, April 1985

John R. Rumble, Jr.

Review of Computerized Information System Development, DOE/ASME/NBS Tribology Data Workshop, NBS, Gaithersburg, MD, July 1985

John R. Rumble, Jr.

Computerized Materials Data - A Progress Report, 1985 National Meeting of AIChE, Seattle, WA, August 1985

John R. Rumble, Jr.

Building In-House Chemical Databases, Chemical Information Symposium of ACS National Meeting, Chicago, IL, September 1985

John R. Rumble, Jr.

Information Science and Materials Data, Plenary Lecture, CODATA Materials Data Workshop, Schluchsee, FRG, September 1985

John R. Rumble, Jr.

Need for ASTM Standard Development Activity, Planning Meeting on Materials Property Data at ASTM, Philadelphia, PA, October 1985

John R. Rumble, Jr.

The Changing Nature of Technical Information, Advanced Technology Update Symposium, Materials Week '85, Toronto, Canada, October 1985

John R. Rumble, Jr. and Jack H. Westbrook

Computerization of Military Handbook 5, Mil-Handbook 5 Committee, Savannah, GA, October 1985

John R. Rumble, Jr.

Using Computers for Engineering Data, ASIS '85 Annual Meeting, Las Vegas, NV, October 1985

John R. Rumble, Jr.

Introduction to Bedford Mark-up, NBS, Gaithersburg, MD, April 1985

Constance L. Seymour

Current Status and Future Trends in Thermophysical Property Research, Spring National AIChE Meeting, Houston, Texas, March 1985.

Howard J. White, Jr.



Thermodynamic Data Bases in the U.S. National Standard Reference Data System, Paris, France, The First CODATA Symposium on Chemical Thermodynamic and Thermophysical Properties Data Bases, Paris, France, September 1985.

Howard J. White, Jr.

Comprehensive, Consistent Thermodynamic Tables: A report on the activities of CODATA, The First CODATA Symposium on Chemical Thermodynamic and Thermophysical Properties Data Bases, Paris, France, September 1985.

Howard J. White, Jr.

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIPJudith T. Calabrese

Bedford Composition System Users Group

Alice A. Dugan

NML Administrative Council

NML Women's Personnel Panel (NBS)

Sherman P. Fivozinsky

Intragency Atomic and Molecular Physics Coordinating Group

NBS Discussion Group on Atomic Physics (steering committee)

Joint Committee on Atomic and Molecular Physical Properties (JCAMP),  
Executive committee-APS representative.  
Chairman, Nominations Committee

DOC Productivity Task Force on Information

AAPM Medical Physics Data Group

Chairman, Organizing Committee, 1987 International Workshop on Atomic Data  
for Fusion and Astrophysics

David R. Lide, Jr.

1985 Herbert P. Broida Prize Committee, APS (Chairman)

American Institute of Physics (AIP Publication Board)

Committee on Nomenclature, 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)

Physical Chemistry Division, IUPAC (President)

Committee on Chemical Databases, IUPAC (Chairman)

Advisory Council, Engineering Information, Inc.

Advisory Committee, Particle Data Center

Bettijoyce B. Molino

NBS User Committee for Scientific Computing

NBS PC Users Committee

NBS National Measurement Laboratory Women's Personnel Panel

ACS Division of Chemical Information - Treasurer

ACS Division of Chemical Information - Long-Range Planning Committee

ACS Committee on Science - Task Force on Scientific Numeric Data

CODATA Task Force on a Referral Database

Bedford Composition System Users Group

John R. Rumble, Jr.

ASTM Committee E-42 Surface Analysis

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

Peer Review, DOE Office of Oil, Gas, Shale and Coal Liquids Information System

Metal Properties Council Task Group of the National Materials Property Data Network

Chairman - User Needs Committee

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

Organizing Committee, Corrosion Data Workshop

Steering Committee, Workshop on Materials Data Resources for the Petroleum Industry

Organizing Committee, Computerizing Materials Data - A Workshop for the Database Industry

Constance L. Seymour

Bedford Composition Systems Users Group

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)



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.

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.

Collection and publication of standard reference data.

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.

Standards, etc. Publication in Federal Register.

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).

Sale of reference data. Cost recovery.

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

31 Stat. 1449; Ante, p. 34. U. S. copyright and renewal rights. 61 Stat. 655; 76 Stat. 446.

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

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

Appropriation.

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

Short title.

SEC. 8. This Act may be cited as the "Standard Reference Data Act."  
Approved July 11, 1968.

---

LEGISLATIVE HISTORY:

HOUSE REPORT No. 260 (Comm. on Science and Astronautics).

SENATE REPORT No. 1230 (Comm. on Commerce).

CONGRESSIONAL RECORD:

Vol. 113 (1967): Aug. 14, considered and passed House.

Vol. 114 (1968): June 13, considered and passed Senate,  
amended.

June 27, House concurred in Senate  
amendments.

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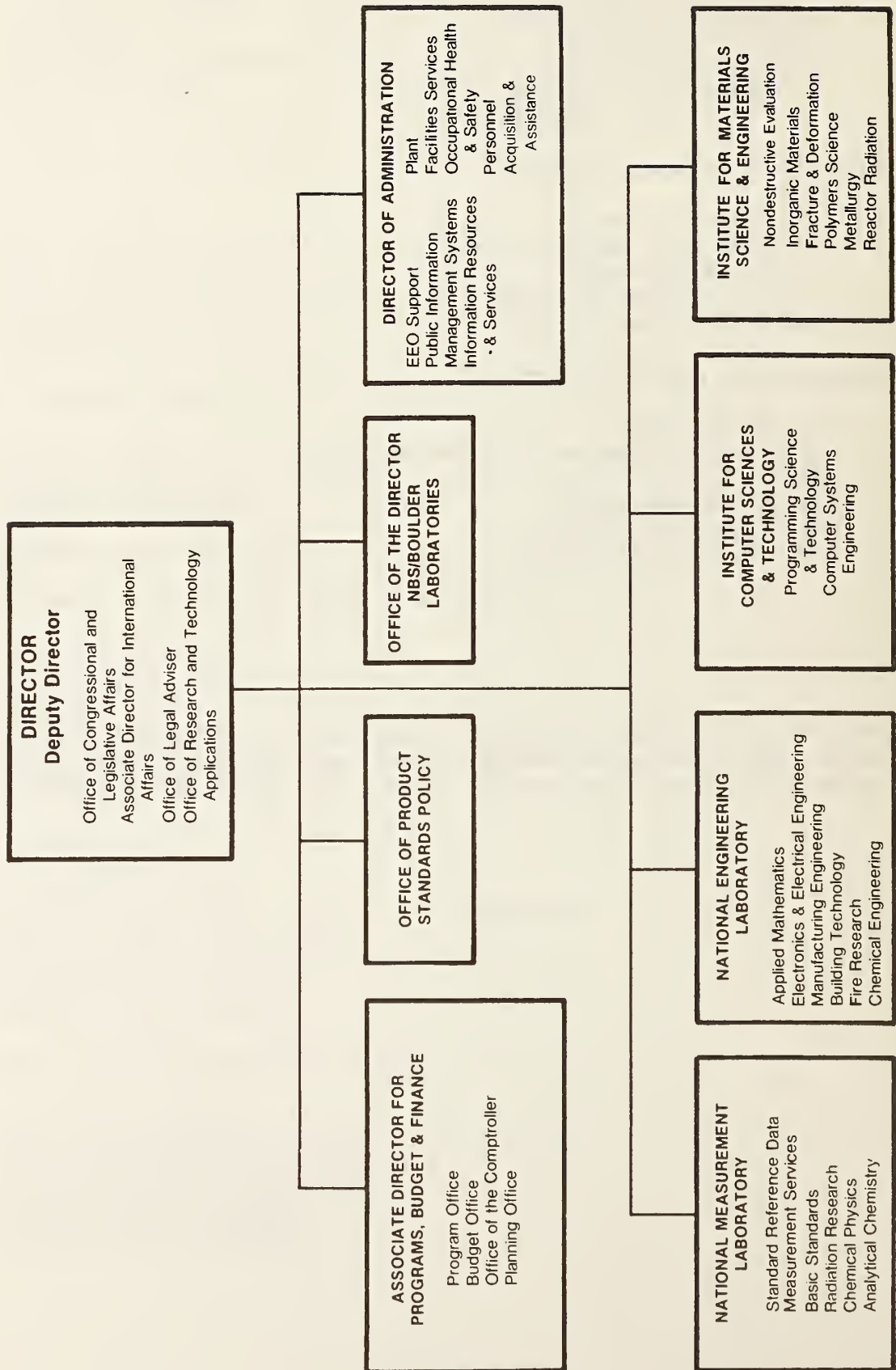
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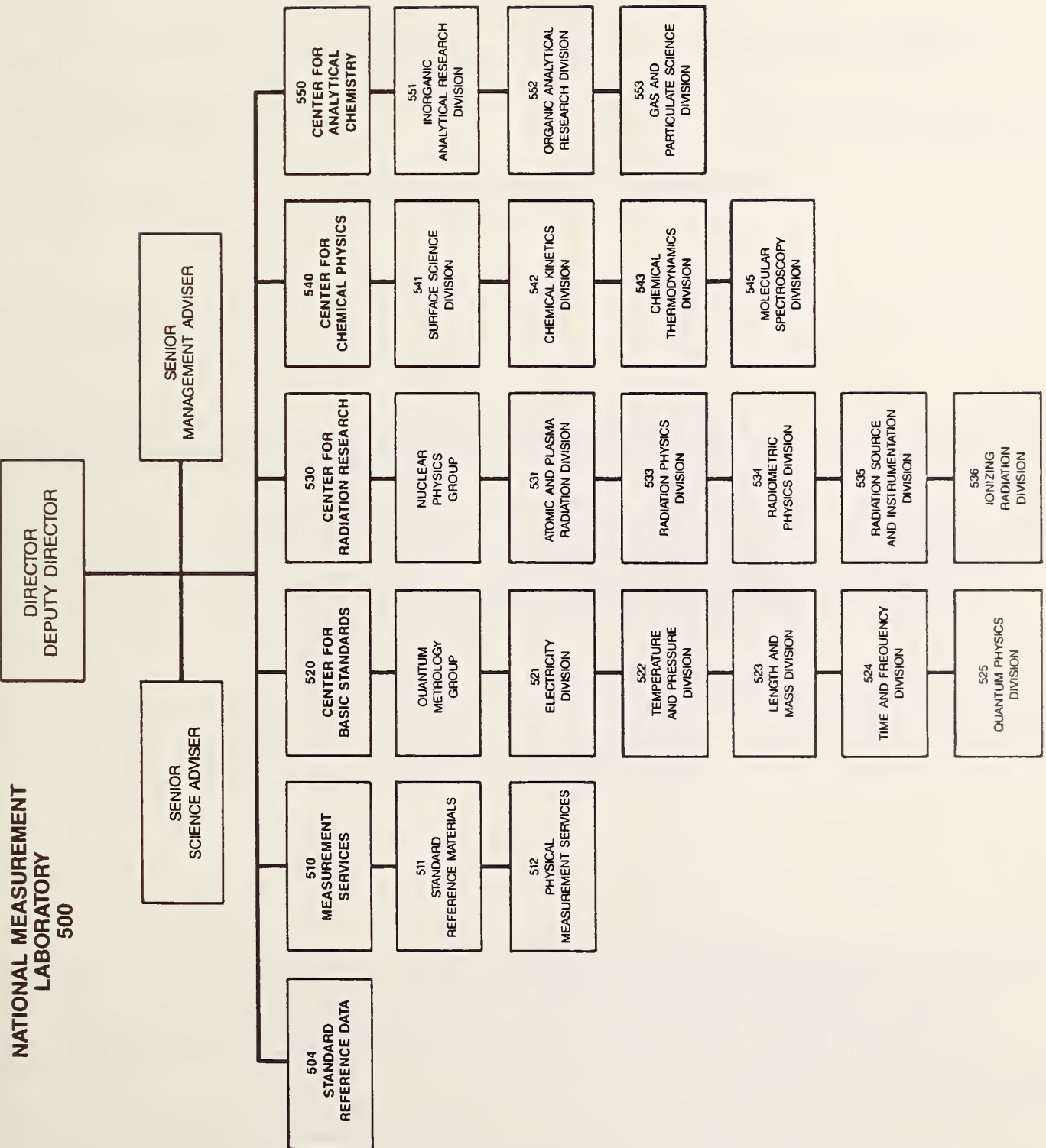
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