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T Technical Activities 1989

Standard Reference Data Program

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ABSTRACT

Standard Reference Data is a program office in the Technology Services, National Institute of Standards and Technology. Standard Reference Data develops and disseminates publications and databases of critically evaluated physical, chemical, and materials properties of substances. These publications and databases are available through NIST and private publications, on magnetic tape, PC diskettes, and from on-line retrieval systems.

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 1989.

Key words: Chemical data; data compilation; evaluated data; materials properties data; numerical database; physical data; standard reference data; technical activities 1989.

INTRODUCTION

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. Other outputs, such as annotated bibliographies, data collections, 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 (since renamed the National Institute of Standards and Technology [NIST]) 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 NIST 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. (See Appendix G.) 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 NIST, 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 engineering materials (alloys, ceramics, etc.) whose composition may vary only within clearly stated ranges. While these definitions leave many borderline cases, the overall intent is to concentrate the effort on intrinsic properties that are clearly defined in terms of accepted physical theory and substances whose composition and history are so well known as to justify evaluation of the data. Biological properties and data relating to large natural systems (e.g., the atmosphere, the oceans) also fall outside the program.

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

The principal output of the program consists of compilations of evaluated data and critical reviews of the status of data in particular technical areas.

Evaluation of data implies a careful examination, by an experienced specialist, of all published measurements of the quantity in question, leading to the selection of a recommended value and 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 magnetic tape and diskettes.

Journal of Physical and Chemical Reference Data - A bimonthly journal containing data compilations and critical data reviews, published for the National Institute of Standards and Technology by the American Institute of Physics and the American Chemical Society. [This journal was published on a quarterly basis through 1989.]

NIST publication series (such as Technical Notes, Special Publications, etc.) distributed by the Superintendent of Documents, U.S. Government Printing Office.

Publications of technical societies and commercial publishers.

Written and verbal responses by SRD and individual data centers and data projects to inquiries for specific data.

PROGRAM STRUCTURE

Current numeric activities in NIST Standard Reference Data are carried out in 21 data centers and approximately 40 short-term projects located in the technical divisions of NIST 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:

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

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

Physics Data - Includes data on atomic, molecular, and nuclear properties, and spectral data utilized for chemical identification. Since comprehensive coverage of all properties and materials of importance in these three program areas is not feasible, Standard Reference Data (SRD) 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 following sections.

In addition to its planning and coordinating role, SRD is responsible for dissemination of the results from the projects that it supports. The evaluated data are made available in both printed and computer-readable form. Response to specific inquiries for data directed to SRD and the individual data centers forms another dissemination mode. There are two additional groups in SRD responsible for aiding in the dissemination process.

Data Systems Development Group - Supports the data centers' work with computer equipment and software, as well as programming assistance; processes evaluated data from magnetic media writing and evaluating databases and typesetting publications to be distributed by SRD.

Reference Center - Delivers to the technical community the results of scientific efforts conducted under the SRD Program, including data compilations in both printed and electronic form.

The current thrust of each group is also described in the following sections.

Eugene S. Domalski, Program Manager

The Chemical Data Program refers primarily to data describing the properties of individual substances and mixtures and data describing the properties of chemical reactions between substances. The properties include: physical properties (such as density), equilibrium and thermodynamic properties (such as equilibrium constants and heat capacities), transport properties (such as viscosity and thermal conductivity), and time-dependent properties (such as rate constants). Thermodynamic and time-dependent properties have applications to chemical reactions as well as individual substances and mixtures.

The descriptive data on substances used in analysis and identification and in selection of materials based on their predicted behavior are not covered in this section. To some extent, these are covered in the section on Physics Data, where all types of spectral data are covered, and in the section on Material Properties Data, where a variety of physical and mechanical property data are covered. The latter section also covers corrosion, a consequence of complex mechanical and chemical behavior, some facets of which are covered by data in this section. Description of phase behavior via phase diagrams also includes the thermodynamic data for the substances involved, although it is covered largely under Material Properties Data. As a result, a reader interested in a specific type of chemical data should investigate all three sections to determine the extent of the coverage.

Structure of the Program

The annual activities of the individual Data Centers and Data Projects are described in the section entitled Data Center Reports. Data Centers are continuing in nature. Their staffs take responsibility for coverage of the data in their fields of specialization and produce an ongoing series of products which provide critically evaluated reference data in the field in question. Data Projects are similar in character. However, they are of shorter term and are directed at one or a few specific products. Lists of the data centers and projects are given in Tables 1 and 2, respectively.

Some centers are listed more than once since their coverage spans more than one principal area. The detailed activities of the data centers and data projects are covered in separate writeups elsewhere in this report. The large data centers often receive support from more sources than Standard Reference Data. Thus, descriptions of centers' activities will in general cover more subjects than those directly supported. In fact, one center, The National Center for the Thermodynamic Data of Minerals (U.S. Geological Survey), receives no direct support from SRD, but is recognized as an important participant in the National Standard Reference Data System.

Table 1

Data Centers in the NSRDS Program for Chemical Data

Aqueous Electrolyte Data Center	NIST, Gaithersburg
Chemical Kinetics Data Center	NIST, Gaithersburg
Chemical Thermodynamics Data Center	NIST, Gaithersburg
Fluid Mixtures Data Center	NIST, Boulder
Ion Kinetics and Energetics Data Center	NIST, Gaithersburg
Molten Salts Data Center	Rensselaer Polytechnic Inst.
National Center for the Thermodynamic Data of Minerals	U.S. Geological Survey
Thermodynamic Research Center	The Texas A&M University

Table 2

Data Projects in the NSRDS Program for Chemical Data

Thermophysical Properties Data for Fluids, University of Maryland
Equations of State for Mixtures of Argon, Nitrogen, Oxygen and of Air,
University of Idaho
International Center for the Systematic Correlation and Dissemination of
the Transport Properties of Fluids, Brown University
Properties of Polar Fluids, NIST, Gaithersburg
Design Institute for Physical Properties Data, AIChE
Properties of Helium, University of Oregon
Application of Expert Systems to Critical Evaluation of Thermophysical
Property Data, Texas A&M Research Foundation
Data on Aqueous Electrolytes, University of Delaware
Gibbs Energies of Formation for Krebs's Cycle and Related Compounds,
University of California, San Diego
A Centralized Database for Thermodynamic Data on Lipid Mesomorphic Phase
Transitions and Miscibility, Ohio State University
Properties of Transition Metal Coordination Complexes, Boston University
OH Radical Reactions with Organic Compounds, University of California,
Riverside

Cooperative Activities

Cooperative activities play a major role in the program for several reasons. There is little value in competitive evaluation programs since a primary purpose for developing evaluated reference databases is to provide users with a common source of data to enhance comparability and consistency in calculations involved in a wide variety of uses, an example being custody transfer of carbon dioxide. Multiple sources of reference data for the same property create confusion and unproductive work. Furthermore, funding and skilled personnel for reference-data activities are severely limited throughout the world.

The cooperative activities can be divided loosely into national and international parts. The primary national activities involve the AIChE Design Institute for Physical Property Data (DIPPR) which is a cooperative organization of chemical companies (primarily, but not exclusively, US companies). DIPPR carries out data evaluation and experimental measurements to provide reference data for the chemical industry. SRD and DIPPR cooperate in a number of ways. SRD is one of many sponsors of DIPPR. SRD carries out selected projects for DIPPR and acts as distributor for automated products for DIPPR. SRD also cooperates in a less formal way with the data programs of the American Petroleum Institute and the Gas Processors Association, and ASME through its Research Committee on the Properties of Steam.

Major international cooperative activities are carried out through CODATA, the International Union of Pure and Applied Chemistry (IUPAC), and the International Association for the Properties of Steam (IAPS). Dr. H. J. White, Jr. (NIST, Retired) is currently serving as a consultant to aid in our participation in these three organizations, as well as in DIPPR and ASME (as mentioned above).

The CODATA Task Group on Chemical Thermodynamic Tables is an international organization involved in preparing a thermodynamically consistent set of tables for formation properties at the standard conditions and thermal functions for a wide range of inorganic substances and their solutions in water. Preparation of these tables involves scientists in four countries on a regular basis and others depending on their interest in the substances involved. New automated techniques had to be developed to make such a decentralized method of operating feasible. Two books from this task group have been published, and a third major effort is underway. The Task Group also cooperates with another CODATA Task Group on Geochemical Thermodynamic Data and a committee of the Organization for Economic Co-operation and Development (OECD).

Cooperation with IUPAC is centered in the Subcommittee on Thermodynamic Tables and the Subcommittee on Transport Properties of the Commission on Thermodynamics. For many years the Subcommittee on Thermodynamic Tables has sponsored the Thermodynamic Tables Project at Imperial College. The project has published the series, International Thermodynamic Tables of the Fluid State, several of which have involved formulations developed in the OSRD program. A volume on ethylene, the final result of an industry-NBS project on the thermodynamic properties of ethylene was published in December 1988. The subcommittee has also produced other products which do not involve the tables project at Imperial College. The Subcommittee on Transport Properties prepares standards and evaluated data on the transport properties of fluids. More detail on its activities is given elsewhere in this report.

The cooperation with IAPS is of many kinds. IAPS is involved with the production of reference data on the properties of water itself, as a working fluid, and on the properties of aqueous solutions which are involved in the power cycle used in generating electricity and can participate in a variety of corrosion and deleterious interactions with the materials of the machinery. Some of the formulations for water endorsed by IAPS have been produced through

SRD, and the work on solutions is closely related to that of the Aqueous Electrolyte Data Center and the Properties of Polar Fluids group.

Computerization and Automation

A major, and increasing, factor in the activities of the Standard Reference Data Program is automation. Several types are involved. Individual data centers usually have large holdings of bibliographic references, abstracts of relevant articles, lists of unevaluated experimental data, as presented by the original author or converted to a common set of units, temperature scale, reference base, etc., which are most efficiently kept and handled in computerized files. They also tend to have substantial needs for software programs, a common example being a non-linear regression package which can be used to determine the value of an expression which results from fitting to data for several properties simultaneously.

In the cooperative programs there is more and more need for the ability to transfer various files from center to center. This may involve transfer by tape or disk but increasingly involves direct computer-to-computer electronic transfer.

Automation is increasingly involved in producing final outputs. Camera-ready tables may be submitted in magnetic form to avoid typesetting and subsequent detailed proofreading. Finally, there is an increasing demand for automated databases for a wide variety of uses. These characteristically involve numerical data, or generating equations for them, and software to aid the user in retrieving the data wanted.

Output

Some noteworthy publications which have resulted from SRD sponsorship during FY 1989 are:

Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups. II. Pyrene Series, Naphthopyrene Series, and Coronene Series, R.A. Alberty, M.B. Chung, and A.K. Reif, J. Phys. & Chem. Ref. Data 18, 77 (1989).

Solubility of Simple Apolar Gases in Light and Heavy Water at High Temperature: A Critical Assessment of Data, R. Fernandez-Prini and R. Crovetto, J. Phys. & Chem. Ref. Data 18, 1231 (1989).

Estimation of the Thermodynamic Properties of Hydrocarbons at 298.15 K, E.S. Domalski, J. Phys. & Chem. Ref. Data 17, 1637 (1988).

Thermophysical Properties of Methane, D.G. Friend, J.F. Ely, and H. Ingham, J. Phys. & Chem. Ref. Data 18, 583 (1989).

Thermodynamic and Transport Properties of Carbohydrates and Their Monophosphates: Pentoses and Hexoses, R.N. Goldberg and Y.B. Tewari, J. Phys. & Chem. Ref. Data 18, 809 (1989).

The Thermal Conductivity of Nitrogen and Carbon Monoxide in the Limit of Zero Density, J. Millat and W.A. Wakeham, J. Phys. & Chem. Ref. Data 18, 565 (1989).

Thermodynamic Properties of Argon from the Triple Point to 1200 K with Pressures to 1000 MPa, R.B. Stewart and R.T. Jacobsen, J. Phys. & Chem. Ref. Data 18, 639 (1989).

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry: Supplement III. IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry, R. Atkinson, D.L. Baulch, R.A. Cox, R.F. Hampson, Jr., J.A. Kerr (Chairman), and J. Troe, J. Phys. & Chem. Ref. Data 18, 1098 (1989).

Evaluated Chemical Kinetic Data for the Reaction of Atomic Oxygen O(³P) with Sulfur Containing Compounds, D.L. Singleton and R.J. Cvetanovic, J. Phys. & Chem. Ref. Data 17, 1377 (1989).

Gas Phase and Neutral Thermochemistry, S.G. Lias, J.E. Bartmess, J.F. Liebman, J.L. Holmes, R.D. Levin, and W. G. Mallard, J. Phys. & Chem. Ref. Data 17, Supplement No. 1, (1988).

Thermodynamic and Transport Properties of Molten Salts: Correlation Equations for Critically Evaluated Density, Surface Tension, Electrical Conductivity, and Viscosity Data, G.J. Janz, J. Phys. & Chem. Ref. Data 17, Supplement No. 2, (1989).

CODATA Key Values for Thermodynamics, J.D. Cox, D.D. Wagman, and V.A. Medvedev (Hemisphere Publishing Corp., 1989).

One of the newest addition to the list of computerized databases, which are sold and distributed through SRD is that by W.G. Mallard, NIST Chemical Kinetics Databases. It is designed to provide rapid access to kinetic data for gas phase reactions including surveys of the literature for a particular reaction, all reaction of a given species, subsets of all the reactions, and the kinetic data available from a given paper. A highly interactive program allows users to search by reactant or by reference. The database contains more than 2000 separate reactions and 8000 records.

Also available as a computerized database is the Educational DIPPR Data Compilation of Pure Compounds by T.E Daubert and R.P. Danner. This DIPPR database contains data for 100 compounds. For each compound, values are given for 26 single-valued property constants and for 13 properties as a function of temperature. The database can accommodate any MS-DOC or PC-DOS System using 2.0 or later.

MATERIALS PROPERTIES DATA

John Rumble, Jr., Program Manager

Several major milestones were accomplished in 1989 in the Materials Data Program.

- * Release of the NIST X-Ray Photoelectron Spectroscopy Database
- * Completion of ACTIS Tribomaterials I Database
- * Release of the first expert system for a NIST data project (with NACE and MTI)
- * Start of Work on Integrated Tribology Information System
- * Publication of new monographs on Alloy Phase Diagrams
- * Release of a New Corrosion Data Management System

Each of these events represents the culmination of several years of work by the Data Centers and Data Projects that make up the SRD Materials Properties Data Program. The program has five major thrusts as shown in Table 1.

Table 1

SRD Materials Properties Data Program

Structure and Characterization
Physical Properties
Phase Equilibria
Performance Properties
 Corrosion
 Mechanical Properties
 Tribology
Computer Access and Databases

The work is accomplished in a variety of ways. Five ongoing data centers and activities exist: Crystal Data, Alloy Phase Diagrams, Phase Diagrams for Ceramists, Corrosion, and Tribology. Each 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. Work is often jointly funded and, in some cases, substantial amounts of industrial support have been raised for these programs.

Table 2

Major NIST-Outside Data Agreements

<u>Society</u>	<u>Data Area</u>
ASM International	Alloy Phase Diagrams
American Ceramic Society	Phase Diagrams for Ceramists
International Centre for Diffraction Data-JCPDS	Crystal Data
National Association of Corrosion Engineers	Corrosion
American Society of Mechanical Engineers	Tribology
American Society of Lubrication Engineers	Tribology

The Materials Properties Data Program also has a number of short-term evaluation projects that address specific data needs within the framework as given in Table 3. These are done both inside and outside NIST. A major part of the program is to develop the tools and technology for computerizing materials properties data. This requires cooperative efforts with American and international standards organizations. In 1989, great progress has been made.

Structure and Characterization

The structure and characterization of solid materials is a fundamental concern. The identification of unknown substances has always been a major use of evaluated data. The NIST Crystal Data Center has two important tools related to crystalline materials. The NIST Crystal Data File, updated again in 1989, now has data on over 130,000 compounds. The database comes with software to analyze experimental measurements and then search the database for matching entries. Negotiations are in progress to integrate this database directly into diffractometers.

One outgrowth from the NIST Crystal Data File is the NIST/Sandia/ICDD Electron Diffraction Database, released in 1987. Important parameters have been calculated from the NIST Crystal Data File and combined with other data from the ICDD's Powder Diffraction File to make the new Electron Diffraction Database which will soon be incorporated directly into electron diffraction instruments.

Table 3

Active SRD Materials Properties Data Program - 1989

Structure and Characterization

Crystallography

NIST Crystal Data Center
Cambridge Crystallographic Data Centre

Surfaces

ESCA Data Project - Surfax (CA)
Ion Sputtering - NIST
Low-Energy Electron Diffraction - Oregon State University
Molecular Adsorption on Transition Metals - Rutgers University

Physical Properties

Properties of Glassy-Forming Melts - Alfred University
Polymer-Polymer Miscibility Data - Rensselaer Polytechnic
Institute

Phase Equilibria

Alloys

NIST Alloy Phase Diagram Data Center
NIST/ASM Phase Diagram Evaluation Program
V, Nb - Ames Laboratory, Iowa
Cr - University of Wisconsin - Milwaukee
Cu - Carnegie-Mellon University
Alkalis - Thermfact, Montreal
Fe - ASM International

Ceramics

NIST Phase Diagrams for Ceramists Data Center

Corrosion

NIST Corrosion Data Center
NIST/NACE Corrosion Data Program
Crevice Corrosion of Stainless Steels - LaQue Center - North
Carolina
Field Test Corrosion Data - LaQue Center - North Carolina

Mechanical Properties

Creep and Stress Rupture - Materials Properties Council
Fracture Toughness of Aluminum Alloy - MPD Network
Fatigue Crack Propagation of Metals - University of Tulsa

Tribology

Tribology Information Activity - NIST

The characterization of surfaces is the other major component of this part of the program. The NIST X-Ray Photoelectron Spectroscopy Database has been released to the public and is already being widely used. Data on over 13,000 compounds are included and the PC database features an easy-to-use interface. Charles Wagner of Surfax, Inc. did an outstanding job on this database.

The SRD compilation for low-energy electron diffraction (LEED) has been incorporated into a database that is in the testing stage. LEED is a widely used technique, and this database will be widely used too. The project on ion-sputtering data is in the last stages of completion. A new project on surface coverage of adsorbed molecules was started in 1988.

Physical Properties

Very little effort is going on in this area at present. Discussions on data evaluation work for new high T_c superconductors have been held, but no projects have been formulated.

Results from data evaluation work done at RPI under the direction of Professor Krause for polymer-polymer miscibility are near completion.

A project on properties of glassy-forming melts is nearing completion of the data evaluation phase. This project is being done in conjunction with the International Commission on Glass and represents the first major data evaluation effort in the area.

Phase Equilibria

NIST, through the Materials Science and Engineering Laboratory (MSEL) and SRD, has two major programs for evaluating phase data for alloys and ceramics. These programs are integrated into the user communities, and considerable progress was achieved last year.

The Phase Diagrams for Ceramists Data Center has completed preparation of Volume 8 of its series Phase Diagrams for Ceramists as part of the joint program with the American Ceramic Society. About 215 critical evaluations and over 900 individual phase diagrams are included.

A PC database and graphics program for ceramics phase diagrams had been completed in 1988. Testing by users has led to improvements, and the database should be completed in 1990.

The ASM/NIST Alloy Phase Diagram Program has continued, and over 1400 binary alloy systems have been evaluated and more than 800 published. Professor Jack Smith of Iowa State, under contract, still is editor for the Bulletin of Alloy Phase Diagrams.

Performance Properties

Corrosion

The NACE-NIST Corrosion Data Program has added new products to their already successful databases, based on the NACE Corrosion Data Surveys. A corrosion data management system has been released and contains the provision for adding proprietary data. Corrosion rate data for sulfuric acid are also available.

In addition, the NACE-NIST has developed an expert system module for materials selection for process and storage equipment in the chemical industry. This project, sponsored by the Materials Technology Institute (MTI), has already produced an expert system for materials in contact with concentrated sulfuric acid that was distributed to MTI's members for their use in 1989.

Mechanical Properties

The SRD effort on mechanical properties data contains several projects to develop techniques and methods for evaluating these data. Since mechanical properties generally result from standardized tests, the assessment of the data quality is different from data on the intrinsic properties of materials.

Several projects are well underway in the areas of fatigue, fracture toughness, and creep- and stress-rupture of alloys.

We take pride in the fact that the compilation of fracture toughness data done by Professor Ebrahimi of the University of Florida, published in the ASTM Journal of Testing and Evaluation in 1988, was selected as the best article of that year.

A new project on evaluation of fatigue crack propagation data for ferrous and nonferrous metals of importance to the automotive industry was started this year at the University of Tulsa. The project will be done in cooperation with the SAE Fatigue Design and Evaluation Committee.

Tribology

A multi-agency program for tribology data, started in 1986, is now well underway. NIST is working together with DOE, NSF, the USAF, ASME, and STLE to improve the quality of tribology data, build databases, and develop expert systems. A formal organization, ACTIS, Inc., has been incorporated.

During 1989, SRD programmers completed the first product of this effort, ACTIS Tribomaterials I Database. This database contains data on over 270 materials commonly used in tribological situations, both unlubricated and lubricated wear. It will be distributed by ACTIS, Inc, starting in early 1990.

Computer Access and Databases

The strong SRD effort to help bring about computerization of materials data has continued, and major accomplishments were achieved in 1989. Several database efforts have already been discussed. Other areas deserve mention.

Standards are a second area of interest. To promote uniformity and compatibility between different materials databases, standards will be needed for identification of materials and reporting of test results. SRD

has vigorously participated in both ASTM Committee E-49 on Computerized Materials Data, the ISO TC184/SC4/WG1 Standard for Exchange of Product Data and the VAMAS Technical Working Group 10 on Factual Materials Databanks.

During 1989, ASTM Committee E-49 has developed and balloted over 20 separate standards, and more are being written. Also, SRD participated in several workshops to advance standards on identification systems for nonmetals, materials data exchange formats, and chemical databases.

Summary

Despite minimal resources, the SRD program on Materials Properties Data remains strong and is moving in new directions. The year 1990 promises even more accomplishments.

PHYSICS DATA

Jean W. Gallagher, Program Manager

The Physics Data Program involves data centers and projects concerning properties associated with the disciplines of physics and physical chemistry. These include fundamental physical constants, atomic and molecular spectroscopy, collisions of low- and medium-energy electrons with gas phase media, the interaction of high-energy photons and charged particles with matter, reactions of radicals and transient species in solution, and energy levels of transient species.

Structure of the Program

The annual activities of the individual data centers are described in the section entitled Data Center Reports. Each Center continues an established "pattern" for a selected body of data defined by clearly stated criteria. A comprehensive bibliography is developed, a library of articles acquired, data are extracted and evaluated, recommended data are entered in a computer file, and an output mode is designed. The output file is designed to print hard-copy tables and/or as a computerized database accessible via a database management system. The output is distributed to the public, and the cycle begins again. A new data body is selected for review. Details of this process vary among the different data centers, but the ongoing pattern is generic. Lists of the data centers and projects are given in Tables 1 and 2, respectively.

The Products

Noteworthy output from the Physics Data Program for FY 1989 include:

1. Completion of "Transition Probabilities for Scandium through Manganese and for Iron Through Nickel." These two Supplements to the Journal of Physical and Chemical Reference Data continue the series started in 1966 with Volume I, "Transition Probabilities for Hydrogen through Ne" and continued in 1969 with Volume II, "Transition Probabilities for Na through Ca." The latter two publications have been designated Citation Classics by the Institute for Scientific Information.
2. Completion of the PC Database, "Electron and Positron Stopping Powers and Ranges" by Stephen M. Seltzer of the Photon and Charged Particle Data Center. This program and database calculates the stopping powers (collision, radiative, and total), Continuous Slowing Down Approximation (CSDA) ranges, density-effect corrections, and bremsstrahlung yields at energies from 1 keV to 10 GeV and for any material that can be designated by a chemical formula.
3. Development of an Atomic Spectra Database which will contain wavelengths, energy levels, and transition probabilities for all atoms and atomic ions continues. Internal agreement on a linear notation to describe all atomic states was reached. Capability of entering data

directly into the database and retrieving on a variety of characteristics was developed.

4. A major article "Microwave Spectral Tables. III. Hydrocarbons, CH to C₁₀H₁₀" was completed and appeared in the Journal of Physical and Chemical Reference Data.

5. A "Bibliography of Electron Swarm Data, 1979-1989" was completed.

6. An informal Workshop on Atomic Physics Databases was held at NIST in March 1989.

These data products are typical outputs from the ongoing efforts of the SRD Physics Data Program which provides a steady stream of reliable data evaluations in both hard copy and computerized format. Resources have limited expansion of activity into new areas where SRD involvement is appropriate such as molecular energy levels and molecular transition probabilities, and resonance ionization mass spectroscopy schema.

Data center staff members have remained active participants in national and international data programs such as the International Atomic Energy Agency, IUPAC, the International Commission on Radiation Units and Measurements, CODATA, the Consultative Committee on Electricity, and the AIP Committee on Numerical Databases.

A search is presently being conducted for a Director for the Atomic Collision Cross Section Data Center at the Joint Institute of Laboratory Astrophysics, the position vacated by the transfer of Jean Gallagher to Standard Reference Data Program.

Table 1
Data Centers in the NSRDS Program for Physics Data

Atomic Energy Levels	NIST, Gaithersburg
Atomic Transition Probabilities	NIST, Gaithersburg
Atomic Collision Cross Sections	JILA, Boulder
Molecular Spectra	NIST, Gaithersburg
Photon and Charged Particle	NIST, Gaithersburg
Radiation Chemistry Data Center	Notre Dame University
Fundamental Constants	NIST, Gaithersburg

Table 2
Data Projects in Physics Program

Energy Levels of Transient Molecules,	NIST, Gaithersburg
Electron Collisional Data for Plasma Processing and Modeling (Univ. of Colorado)	NSF funding
An Evaluated Compilation of Ion Solvation Energetics (Univ. of Tennessee)	NSF funding
Resonance Ionization Spectroscopy (Univ. of Tennessee)	NSF funding

The Data Systems Development Group (DSDG) has expanded in two significant directions.

First, while continuing to review and refine the databases built in the data centers, we have built distributable databases ourselves. For example, the X-ray Photoelectron Spectroscopy database is on the market with current sales of 34 since November. The Fundamental Constants database was built as a prototype for our collaboration with the American Institute of Physics (AIP). This database will be test marketed by AIP in FY 1990. The Vibrational and Electronic Energy Levels of Small Polyatomic Transient Molecules database will be on the market next month. A lipids database is in its early stages. These data were compiled and evaluated in data centers or under our grants proposal program, but the interactive access was built in-house by DSDG staff.

Second, the numeric and bibliographic databases in the Oracle database management system are being expanded and are contributing to the dissemination of our data in the following ways. The Atomic Energy Levels System produces tapes of data for distribution and the data can be retrieved directly in typeset format for publications. The NBS Tables of Chemical Thermodynamic Properties are maintained in this database system, and retrievals are made to provide updated files for the online retrieval system at STN. The Ion Energetics Data Center is prototyping a data entry program utilizing the SQL*Forms tool which facilitates elaborate error checking at input. This error checking is also used extensively in the Atomic Spectroscopic Database. The ability to clean up errors in the data before they get hidden in database files is a great asset. The JANAF Thermochemical Tables files are currently being moved into the ORACLE system for maintenance and subsequent production of updates.

Publications

DSDG staff involved with publications have concentrated on programmatic conversion of other magnetic media files to Bedford format for typesetting of JPCRD, Technical Notes, Monographs, and SRD Newsletters. We have also started producing the database documentation users' guides which are distributed with our databases through this system for inclusion in SRD 3-ring notebooks which are of the same size as most PC products.

JPCRD, for which we prepare 30 percent of the papers, will now be printed 6 times per year, instead of 4 times per year. This increase cuts our preparation time from 3 to 2 months for each volume. As a result we are investigating various options for reducing the processing time for all manuscripts.

The recent acquisition of a Macintosh work station is proving to be an excellent environment for preparing graphics illustrations for the papers and documents we publish.

Computer Systems

The Data Systems Development Group supports and manages: the HP UNIX mini-computer for data processing and maintenance of data systems (i.e., Crystal, NBS Tables of Chemical Thermodynamic Properties, the JANAF Thermochemical Tables, Atomic Energy Levels, Atomic Transition Probabilities); the Bedford UNIX system for publications; the development PC's (286 and 386 computers) for the production and review of marketable PC databases; and the SRD staff's PC's, including those used for database reproduction. In addition, we have assumed responsibility for maintenance and backup procedures for the HP 1000 (RTE-A) minicomputer in the Chemical Thermodynamics Data Center. The data files on the HP 1000 will be transferred, over the next two years, to the SRD computer and PC's. We continue to utilize the CDC supercomputer for production of the several versions of the Mass Spec tapes. This has our very able staff spread over a wide range of operating systems and equipment. Our communications knowledge and file transfer abilities have expanded significantly. We have installed local area networks (LAN's) in both the database building section and the publishing section of our operations. The database LAN is connected to the new NIST high-speed backbone, and we plan to link the publishing section to that backbone in the spring, followed by the reference center. This will facilitate the transfer of databases and documentation from development in Data Systems to distribution through the reference center and to publication of documentation on the Bedford.

Included in the database section network is our Macintosh. We have started expanding into the Macintosh environment. A private company working on a cooperative project with the Thermophysics Division requested the Macintosh versions of some of their programs. Three thermophysics databases are in varying stages of conversion. We can make programs run in that environment but we have a great deal of work to do before they will be "Mac like." Finally, Data Systems is experimenting with Soft PC, a software package which allows Mac's to run DOS programs.

We have also installed the PC MKS environment (UNIX) and OS2 to allow testing of all databases while those operating systems are resident on a system.

Electronic Products

Three databases recently released are the X-ray Photoelectron Spectroscopy Database, the student version of the Design Institute for Physical Properties (DIPPR) Thermophysical and Transport Properties of Pure Compounds, and the Electron and Positron Stopping Powers and Ranges program.

The X-ray and Gamma-ray Attenuation Coefficients and Cross Sections program was significantly modified by Data Systems such that it is now operated through a menu system, and the tables of calculated results can now be graphed on the screen.

Several programs and/or data compilations which have been received from the data centers or data projects are in the final stages of review of both the interactive PC operation and documentation. These data compilations are: Thermophysical Properties of Hydrocarbon Mixtures; Properties of Refrigerants and Refrigerant Mixtures; Positive and Negative Ion Energetics; Thermodynamic Properties Estimator; Vibrational and Electronic Energy Levels of Small Polyatomic Transient Molecules; Thermodynamic and Transport Properties of Molten Salts; and Biological Macromolecule (Protein) Crystallization.

The above products are all designed for PC's and include interactive software. We are also preparing a new data compilation of Atomic Transition Probabilities data which is being provided on diskettes.

REFERENCE CENTER

The Reference Center acts as a focal point for technical inquiries on data compilations in printed and electronic form, including The Journal of Physical and Chemical Reference Data (continuing under the leadership of Dr. David R. Lide as editor) and The NIST Standard Reference Database Series from scientists in industry, government, and the academic community. As distribution center for the databases, Reference Center personnel negotiate licenses and process and receive database monies. PC databases, including various updates and documentation, are reproduced in the Reference Center. Reference Center personnel actively promote SRD products by designing, writing, and typesetting various promotional products, including SRD Newsletters, brochures, publications lists and flyers. Extensive mailing lists of customers are also maintained in the Reference Center.

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

Inquiries Received in SRD

(Does not include inquiries received by data centers)

<u>Year</u>	<u>Number</u>
1981	657
1982	613
1983	1022
1984	616
1985	623
1986	926
1987	2172
1988	2010
1989*	2905

*Projected to end of year

Publications in 1989

<u>Series</u>	<u>Pages Published</u>	<u>Titles Published</u>
JPCRD, Vol. 18	2188	20
Data Compilations from other publishers	8222	4
Other Publications in NBS Series	478	1
Bibliographies and indexes from other publishers	<u>897</u>	<u>4</u>
Total	11785	29

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
1986	2019	383
1987	1906	2222
1988	3926	1376
1989*	3128	2026

*Projected to end of year

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
8/1986	1087
9/1987	1076
9/1988	1047
9/1989	991

DATABASE SALES
January 1, 1989 -- December 8, 1989

NIST/EPA/MSDC Mass Spectral Database Version 1.0	53
Upgrade from Version 1.0 to Version 2.0 (PC Version Mass Spectral Database)	21
NIST Chemical Thermodynamics	3
NIST Electron and Positron Stopping Powers (EPSTAR)	3
NIST X-ray and Gamma Ray Attenuation Co- efficients and Cross Sections (XGAM)	12
NIST Activity and Osmotic Coefficients of Aqueous and Electrolyte Solutions (GAMPHI)	3
NIST Thermophysical Properties of Water	3
DIPPR Data Compilation of Pure Compound Properties	7
Upgrade to Version 4.0-DIPPR Data Compilation of Pure Compound Properties	10
Student DIPPR	8
NIST Thermophysical Properties of Fluids	20
NIST JANAF Thermochemical Tables	9
NIST Thermophysical Properties of Mixtures (DDMIX)	8
NIST Chemical Kinetics	215
NIST X-ray Photoelectron Spectroscopy	<u>34</u>
	409

PUBLICATIONS IN 1989

Journal of Physical and Chemical Reference Data, Volume 18

No. 1

Standard Electrode Potentials and Temperature Coefficients in Water at 298.15K

Steven G. Bratsch

Cross Sections for Collisions of Electrons and Photons with Oxygen Molecules
Y. Itikawa, A. Ichimura, K. Onda, K. Sakimoto, K. Takayanagi, Y. Hatano,
M. Hayashi, H. Nishimura, and S. Tsurubuchi

Thermal Conductivity of Refrigerants in a Wide Range of Temperature and Pressure

R. Krauss and K. Stephan

Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups. II. Pyrene Series, Naphthopyrene Series, and Coronene Series

Robert A. Alberty, Michael B. Chung, and Andrea K. Reif

Cross Sections for K-Shell x-Ray Production by Hydrogen and Helium Ions in Elements from Beryllium to Uranium

G. Lapicki

Rate Constants for the Quenching of Excited States of Metal Complexes in Fluid Solution

Morton Z. Hoffman, Fabrizio Bolletta, Luca Moggi, and Gordon L. Hug

No. 2

The Thermal Conductivity of Nitrogen and Carbon Monoxide in the Limit of Zero Density

J. Millat and W. A. Wakeham

Thermophysical Properties of Methane

Daniel G. Friend, James F. Ely, and Hepburn Ingham

Thermodynamic Properties of Argon from the Triple Point to 1200 K with Pressures to 1000 MPa

Richard B. Stewart and Richard T. Jacobsen

Thermodynamic Properties of Dioxygen Difluoride (O_2F_2) and Dioxygen Fluoride (O_2F)

John L. Lyman

Thermodynamic and Transport Properties of Carbohydrates and Their Monophosphates: The Pentoses and Hexoses

Robert N. Goldberg and Yadu B. Tewari

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry: Supplement III.

R. Atkinson, D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr (Chairman), and J. Troe

No. 3

Octanol-Water Partition Coefficients of Simple Organic Compounds

James Sangster

Evaluation of Data on Solubility of Simple Apolar Gases in Light and Heavy Water at High Temperature

Roberto Fernandez Prini and Rosa Crovetto

Microwave Spectral Tables. III. Hydrocarbons, CH to C₁₀H₁₀

F. J. Lovas and R. D. Suenram

No. 4

A Fundamental Equation for Water Covering the Range from the Melting Line to 1273 K at Pressures up to 25 000 MPa

A. Saul and W. Wagner

Toluene Thermophysical Properties from 178 to 800 K at Pressures to 1000 Bar

Robert D. Goodwin

Reduction Potentials of One-Electron Couples Involving Free Radicals in Aqueous Solution

Peter Wardman

Photoemission Cross Sections for Atomic Transitions in the Extreme Ultraviolet due to Electron Collisions with Atoms and Molecules

P. J. M. van der Burgt, W. B. Westerveld, and J. S. Risley

Other Publications in NIST Series

Tables for the Thermophysical Properties of Methane, NIST Tech Note 1325

Daniel G. Friend, James F. Ely, and Hepburn Ingam

Data Compilations from Other Publishers

CODATA Key Values for Thermodynamics, J.D. Cox, D.D. Wagman, V.A. Medvedev, NY: Hemisphere Publishing Corp., 271 pp. (1989)

Measurements of Electron Impact Optical Excitation Functions, D.W.O. Heddle, J.W. Gallagher, Rev. Mod. Phys., Vol. 61, 221 (1989)

A Simplified Representation for the Thermal Conductivity of Fluids in the Critical Region, G.A. Olchowy, J.V. Sengers, Int. J. Thermophys., Vol. 10, 417 (1989)

The Wiley/NBS Registry of Mass Spectral Data, Volumes 1-7, F.W. McLafferty, D.B. Stauffer, NY: John Wiley and Sons, 7313 pp. (1989)

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Vol. 22, 1989-Rad. Chem. 21, Notre Dame, IN, Radiation Chem. Data Center, U. of Notre Dame, 32 pp. (1989)

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Vol. 22, 1989-Rad. Chem. 22, Notre Dame, IN, Radiation Chem. Data Center, U. of Notre Dame, 498 pp. (1989)

Mossbauer Effect Reference and Data Journal, J.G. Stevens, V.E. Stevens, M.A. Goforth, V.L. Coman, C.R. Boss (editors), Moss. Effect Ref. Data J., Vol. 12, Asheville, NC: Moss. Effect Data Center, U. of NC (1989)

PUBLICATIONS SCHEDULED FOR 1990

Journal of Physical and Chemical Reference Data

Standard Chemical Thermodynamic Properties of Isomer Groups of Monochloroalkanes

Robert A. Alberty and Michael B. Chung

Standard Chemical Thermodynamic Properties of Thiaalkane Isomer Groups

Robert A. Alberty, Tae H. Kang, and Ellen Burmenko

The Solubility of Magnetite in Water and Aqueous Solutions of Acid and Alkali

G. Bohnsack, K. Kuhnke, and H. Bohnsack

The Thermodynamics of the Krebs Cycle and Related Compounds

Stanley L. Miller

Chemical Kinetic Data Base for Combustion Chemistry. Part IV: Isobutane

Wing Tsang

The Transport Properties of Carbon Dioxide

V. Vesovic, W.A. Wakeham, G.A. Olchoway, J.V. Sengers, J.T.R. Watson, and J. Millat

Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups III. Naphthocoronene Series, Ovalene Series, and First Members of Some Higher Series

Robert A. Alberty, Michael B. Chung, and Andrea K. Reif

Critical Compilation of Surface Structures Determined by Ion Scattering Methods

Philip R. Watson

Heat Capacities and Entropies of Organic Compounds in the Condensed Phase

E.S. Domalski and Elizabeth Hearing

Energy Levels of Atomic Aluminum with Hyperfine Structure

Edward S. Chang

Thermodynamic Data for Iron from 200 to 3000 K and From 0 to 200 KBAR

John L. Haas, Jr. and Malcolm W. Chase, Jr.

Updated Excitation and Ionization Cross Sections for Electron Impact on Atomic Oxygen

Russ R. Laher and Forrest R. Gilmore

Spectral Data and Grotian Diagrams for Highly Ionized Iron, Fe VIII - Fe XXVI

Toshizo Shirai, Yoshio Funatake, Kazuo Mori, Jack Sugar, Wolfgang L. Wiese, and Yohta Nakai

The Dielectric Constant of Water and Debye-Huckel Limiting Law Slopes

Donald G. Archer and Peiming Wang

Coupled Phase Diagram/Thermodynamic Analysis of the 24 Binary Systems
Yves Dessureault, James Sangster, and Arthur D. Pelton

Benzene: A Further Liquid Thermal Conductivity Standard
M.J. Assael, M.L.V. Ramires, C.A. Nieto de Castro, and W.A. Wakeham

Heat Capacities of C1 to C18 1-Alkanols in Liquid State
Milan Zabransky, Vlastimil Ruzicka and Vladimir Majer

Cross Sections and Swarm Coefficients for H^+ , H_2^+ , H_3^+ , H , H_2 and H^- and H_2
for Energies from 0.1 eV to 10 keV
A.V. Phelps

Cross Sections and Related Data for Electron Collisions with Hydrogen Molecules and Their Ions
H. Tawara, Y. Itikawa, H. Nishimura, and M. Yoshino

Cross Sections for Collisions of Electrons and Photons with Atomic Oxygen
Y. Itikawa and A. Ichimura

Energy Levels of Copper, Cu I through Cu XXIX
Jack Sugar and Arlene Musgrove

The Thermal Conductivity of Methane and Tetrafluoromethane in the Limit of Zero Density
M.J. Assael, J. Millat, V. Vesovic, and W.A. Wakeham

Aqueous Solubility of Organic Chemicals: A Compilation of Experimental Data, Correlations and Predictive Models
N. Nirmalakhandan and R.E. Speece

A Unified Equation of State for H_2O
Philip G. Hill

Rate Constants for Reactions of Peroxyl Radicals in Fluid Solutions
P. Neta, Robert E. Huie, and Alberta B. Ross

SRD DATA CENTERS AND DATA PROJECTS

The numeric data programs, and their major FY 1989 accomplishments, are listed in the following pages. The data centers are listed first, followed by the data projects and grants. For the data centers, a brief description of the objectives of the center is given also. In all cases, SRD money is used to fund their activities (although these centers typically have other sources of monies). For the data projects, a summary of the FY 1989 activity is given, as is their source of funding. The data center and data project activities are discussed in more detail in the NIST Technical Activities Reports of the respective divisions in which the center/project organizationally resides.

ALLOY PHASE DIAGRAM DATA CENTER

Director: E. Neville Pugh
Institute for Materials Science and Engineering, NIST

The Alloy Phase Diagram Center is the technical coordinator for the NIST-ASM Phase Diagram Program.

The Center is responsible for the technical content and editing of the Bulletin of Alloy Phase Diagrams, a joint bimonthly publication with ASM International. The Bulletin has become the prime source of evaluated phase diagrams. Computer graphics software for phase diagrams was developed by NIST and is used by ASM to help produce the Bulletin.

Four monographs on individual binary systems have been published, two of these the result of work by NIST scientists.

AQUEOUS ELECTROLYTE DATA CENTER

Director: David B. Neumann
Center for Chemical Technology, NIST

The Electrolyte Data Center, ELDC, serves as a national and international source of critically evaluated chemical thermodynamic data for aqueous electrolyte systems. It provides temperature, pressure, and concentration-dependent data on activity and osmotic coefficients and excess thermodynamic properties of aqueous salts and salt mixtures. Such data are required in the analysis of chemical and biochemical equilibria and are crucial to the computer simulation of chemical processes occurring in a variety of areas ranging from geology to chemical engineering to biotechnology.

Among the significant accomplishments during the past year are: development of the computer code required to fit experimental measurements over wide ranges of T, P, and x; expansion of the capabilities of the PC version of the Aqueous Thermodynamics Database to accommodate E°-pH diagrams; expansion of the capabilities of the GAMMIX program for the calculation of

activity and osmotic coefficients. This PC database is planned for a FY 1990 distribution.

ATOMIC COLLISION CROSS SECTION DATA CENTER

Director: (Vacant)
Joint Institute for Laboratory Astrophysics
University of Colorado, Boulder, Colorado

The purpose of the JILA Data Center is to compile and evaluate data describing non-reactive collisions of electrons and photons with atoms, ions, and simple molecules.

The comprehensive review article "Cross Sections and Swarm Coefficients for H^+ , H_2^+ , H_3^+ , H, H_2 , and H^- in H_2 for Energies from 0.1 eV to 10 keV" by A. V. Phelps was completed and submitted to the Journal of Physical and Chemical Reference Data.

The Multiphoton bibliography 1983-1986, S. J. Smith, J. H. Eberly and J. W. Gallagher [NBS LP-92, Supp. 5, June 1989] which is a continuation and expansion of the existing collection of references describing studies of the interaction of more than one photon with individual atoms and molecules in the gas phase was completed.

The "Bibliography of Electron Swarm Data" by W. Lowell Morgan covering published data on the transport properties of electron swarms in gases and cross section information derived therefrom during the period from 1979 to mid-1989 was completed.

Work continued on the second part of the review series "Collisional Alignment and Orientation in Atomic Outer Shells. II. Quasimolecular Excitation. N. Andersen, E. Campbell, J. W. Gallagher, I. V. Hertel.

Starting in October, 1989, a search will be conducted for a Director for the Data Center, the position vacated by the transfer of Jean Gallagher to the Standard Reference Data Program Office.

ATOMIC ENERGY LEVELS DATA CENTER

Director: William C. Martin
Center for Atomic, Molecular, and Optical Physics, NIST

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.

An evaluated compilation of wavelengths, energy-level classifications, and Grotrian diagrams for 19 iron spectra is in press at the Journal of Physical and Chemical Reference Data. In addition, a new energy-levels compilation for all 29 copper spectra (Cu I - XXIX) has been completed and

submitted for publication. A separate compilation of the wavelengths and classifications for the spectral lines of 24 of these spectra (Cu VI-XXIX) is almost complete.

Work continues on a compilation of wavelengths and energy-levels classification for silicon spectra in collaboration with workers from the Japan Atomic Energy Research Institute (Ibaraki) and the Institute of Plasma Physics (Nagoya) in Japan.

Plans for FY 1990 include publication of a compilation of energy-level data for all sulfur spectra (S I - XVI), and completion of wavelengths compilations with energy-level classifications for all spectra of the elements silicon, sodium, and magnesium. Work will begin on compiling energy levels for krypton and chlorine.

The first round in the development of an Atomic Spectroscopy Database has been completed. Energy-level entry and retrieval capability have been achieved, and data for approximately 300 spectra have been read into the database. The next step, envisioned for FY 1990, is to develop capability for entry and retrieval of wavelengths, energy-level classifications, and transition probabilities for atomic spectral lines.

ATOMIC TRANSITION PROBABILITIES DATA CENTER

Director: Wolfgang L. Wiese
Center for Atomic, Molecular, and Optical Physics, NIST

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 modeling and analysis, including fusion research, as well as laser physics and astrophysics.

During FY 1989 comprehensive tables of atomic transition probabilities for the elements Sc through Mn and Fe through Ni were published as Supplements 3 and 4 to Volume 17 of JPCRD.

A book chapter entitled "On the Accuracy of Atomic Transition Probabilities" was completed for publication in the Springer Verlag series Lecture Notes in Physics. Tables for Ti, Cr, and Ni including wavelengths, energy levels, and transition probabilities were completed for the "Redbook" series, "Atomic Data for Fusion," put out by Oak Ridge National Laboratory. Involvement continues in the Data Center Network of the International Atomic Energy Agency (IAEA) in Vienna and in "Experts' Meetings" regarding data needs for the plasma edge region.

Plans for FY 1990 include critical evaluation of the transition probabilities of the ten lightest elements (hydrogen through neon). Incorporation of high-accuracy calculated transition probabilities from the Opacity Project into the database is planned. Due to newly available results, new evaluations of Mo, Ba, and Hg are also in progress.

A bibliographical database on transition-probability literature has been developed and several hundred literature references have been entered into this system.

Work is beginning on an Atomic Spectroscopy Database which will allow entry and retrieval of energy levels, wavelengths, energy-level classifications, and transition probabilities for atomic spectral lines.

CHEMICAL KINETICS DATA CENTER

Director: John T. Herron
Center for Chemical Technology, NIST

The goal of the Chemical Kinetics Data Center is to serve as the nation's primary source for evaluated chemical kinetic data. The emphasis is on gas phase processes for which there is a demonstrated need. The approach is to compile all data on gas phase chemical kinetics, and to evaluate specific subsets of this general database. This allows us to concentrate our efforts on those areas of greatest practical interest, while maintaining the ability to move rapidly into new evaluation activities as the need arises. The evaluated and unevaluated databases are also available to outside users.

Evaluated chemical kinetic data are most needed in those areas of science and technology in which computer simulation studies are being used to predict the behavior of large scale, complex chemical systems. Thus, the focus of our evaluation program is in the area of the oxidation of organic compounds, particularly as related to combustion and atmospheric chemistry. This also constitutes the largest active area in experimental chemical kinetics.

Activities over the past year include:

- continued expansion of the evaluated chemical kinetic database for combustion chemistry.
- extension of the original data for methane to include methanol, C₃ alkanes and alkyl radicals, and C₄ alkanes and alkyl radicals. A series of publications are appearing in JPCRD (W. Tsang, Chemical Kinetic Data Base for Combustion Chemistry. Part 3. Propane, J. Phys. Chem. Ref. Data 17, 887 (1988) and W. Tsang, "Chemical Kinetic Data Base for Combustion Chemistry. Part 4. t-Butyl, and i-Butane," J. Phys. Chem. Ref. Data., in press).
- continued support for the NASA stratospheric chemistry program, with evaluation activities in the area of halogen chemistry (in conjunction with the NASA Panel for Data Evaluation and the IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry).
- analysis of dielectric breakdown and chemical vapor deposition (plasma chemistry) with consideration of the thermal stability of sulfur hexafluoride and disulfur decafluoride. The design of a database of evaluated data on reactions in the SF₆/O₂/H₂O system has been completed.

- the most important accomplishment of FY 1989 has been the completion and release for sale of the PC version of the NIST Chemical Kinetics Database. This database is of high interest within the field of chemical kinetics and related applied areas. A highly interactive program allows the user to search by reactants or by reference. The database contains more than 2000 separate reactions and 8000 records.

CHEMICAL THERMODYNAMICS DATA CENTER

Director: Eugene S. Domalski
Center for Chemical Technology, NIST

The Center provides the chemical process industry and related industries with critically evaluated thermodynamically consistent data which can be used to establish the equilibrium constants and enthalpies 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 sciences, metallurgy, and other fields where chemical interactions are important. Research projects in the Center focus on the thermodynamic properties of both inorganic and organic compounds.

The Center surveys the thermodynamic literature and extracts pertinent data with particular emphasis on the active research projects rather than the entire scope of all available thermodynamic property information.

Inorganic Thermochemistry

Thermodynamic properties of selected chemical elements are being studied for the JANAF Thermochemical Tables project. The initial bibliographic portion of this effort has been completed. The data collection and evaluation process is nearing completion. In addition, for the JANNAF Subcommittee on Combustion, the study of the thermodynamic properties of many gaseous species has been completed containing the elements C, H, N, and O. A similar study for NASA is in progress on gaseous chlorine oxides, oxy-halogen acids, and related species.

The Center is cooperating through CODATA, with other centers located in Europe and the United States, to develop thermodynamic tables for iron and its compounds. A similar effort was begun to develop thermodynamic tables for yttrium and its compounds.

Organic Thermochemistry

Continued progress was made in developing schemes for the estimation of the heat capacity, entropy, and formation properties at 298.15 K for species of the type C-H, C-H-O, C-H-N, and C-H-N-O in the crystal, liquid, and gaseous states. Final corrections to: Heat Capacities and Entropies of Organic Compounds in the Condensed Phase. Volume II, were completed.

CORROSION DATA CENTER

Director: David B. Anderson
Institute for Materials Science and Engineering, NIST

The Corrosion Data Center provides scientific and technical coordination to the joint program between the National Association of Corrosion Engineers (NACE) and NIST. The program objective is to enhance the availability of corrosion information through collection, evaluation, and dissemination of performance data on engineering materials exposed to a wide variety of corrosive environments. A key activity is establishment of an evaluated database to serve as the basis for a series of distributed software addressing specific industrial needs.

Two databases, based on published compilations for both metals and nonmetals, have been completed and are being marketed by NACE. Software is also in development for calculation and display of potential -pH stability diagrams in a simplified PC format. Efforts in conjunction with key NACE and ASTM task groups have led to a basis for standardization of corrosion data formats compatible with database management needs for data capture and structuring search strategies to support a diverse user base. The formats will also assure compatibility with other material property databases currently under development.

Multiple data sources have been identified, and programs are underway to capture and compile data for introduction into a centralized database. Efforts have also been initiated, supported by a second NACE Research Associate, to develop expert system modules for materials selection for process and storage equipment with applications in key sectors of the chemical industry. The first module on materials for handling and storing concentrated sulfuric acid will be done in early 1989.

CRYSTAL DATA CENTER

Director: Alan D. Mighell
Institute for Materials Science and Engineering, NIST

The NIST Crystal Data Center collects, evaluates, and disseminates data on solid-state materials. The Data Center maintains a comprehensive database for chemical, physical, and crystallographic information on all types of well characterized substances. Data and specially designed scientific software are made available to the scientific community in three distinct modes: 1) NIST CRYSTAL DATA Distribution Package (1987); 2) International Online Search System; 3) Specialized Database for Electron Diffractionists.

The first product is NIST CRYSTAL DATA, a FORTRAN program (NIST*SEARCH), and accompanying documentation. NIST CRYSTAL DATA contains up-to-date crystallographic data on more than 115,000 materials. Each entry consists of the reduced cell and volume, crystal system, space group symbol

and number, chemical name, chemical formula, literature reference, and other data. NIST*SEARCH software has been designed to be used for the characterization and identification of crystalline materials.

The NIST Crystal Data Center and CISTI's CAN/SND Scientific Numeric Database Service (Canada) collaborate to make the data available through CRYSTDAT. CRYSTDAT is an online, state-of-the-art database search system that can easily be accessed by scientists worldwide.

A new product, designed specifically for electron diffractionists, is now available. This product allows the experimentalist to identify materials using such typical electron diffraction data as elemental information and d-spacings. The database for electron diffraction was prepared in three basic steps. To generate this derivative database, d-spacings (3.6 million) were calculated for all inorganic compounds in NIST CRYSTAL DATA using cell and space group information. These data were then combined with similar data on 10,000 entries from the Powder Diffraction File. Extensive tests using observed electron diffraction data have proved that the database provides a major new analytical tool for electron diffractionists. The generation of this new product was carried out as a collaborative effort between the NIST Crystal Data Center and Dr. Martin Carr of the Sandia National Laboratories.

FLUID MIXTURES DATA CENTER

Director: James F. Ely
Center for Chemical Technology, NIST

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 wide ranges 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 databases which are then disseminated by SRD and other organizations.

The computer package MIPROPS is being distributed by SRD and is available through the on-line services of CAS/STN. The DDMIX computer package, after undergoing substantial technical and software changes, also is available for distribution through SRD. DDMIX has been valuable to industry in the contractual custody transfer of carbon-dioxide-rich mixtures and in engineering design. Upon completion of major improvements in the transport property theoretical model, SUPERTRAPP has been delivered to SRD for testing.

The analysis of the thermodynamic properties of methanol, benzene, and toluene has been completed. While the methanol paper has been already published, the other two contributions are in the review process. A major

critical evaluation of the properties of methane has been completed and was published in JPCRD (J. Phys. Chem. Ref. Data 18, 583-638 (1989)). A companion set of property tables has been published as NIST Technical Note 1325, April 1989. In addition, a critical evaluation on the properties of ethane is in review for JPCRD while a similar work on propane is near completion.

FUNDAMENTAL CONSTANTS DATA CENTER

Director: Barry N. Taylor
Center for Atomic, Molecular & Optical Physics, NIST

The Data Center carries out least-squares adjustments of the fundamental physical constants resulting in the international adoption of recommended sets of constants. The Center also 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 participates in the organization of conferences and/or sessions at conferences relating to the precision measurement-fundamental constants (PMFC) field; administers the NIST Precision Measurement Grant program; and participates in the work of various committees and organizations active in the PMFC field such as the NAS/NRC Advisory Committee on Fundamental Constants and Basic Standards, and the APS Topical Group on Fundamental Laws and Constants.

During FY 89 work related to the new representations of the volt and the ohm, including preparation of related reports and attendance at committee meetings, was carried on. A work schedule which will lead to the completion of the next least-squares adjustment of the fundamental constants by the end of 1992 was developed in collaboration with the International Bureau of Weights and Measures and the CODATA Task Group on Fundamental Constants. Final reports of recommended values and a detailed description of the analysis to be published simultaneously in JPCRD and RMP are planned. Working with the International Standards Organization, a draft document entitled "Guide on the Expression of Uncertainty in Physical Measurements" was prepared.

Plans for FY 90 include (1) preparation of a status report on the fundamental physical constants for presentation at the 1990 Conference on Precision Electromagnetic Measurements; (2) moving the Data Center to larger quarters and organizing and updating the reprint files; (3) organization of sessions on the fundamental constants at various major conferences, and participation in various committees related to the fundamental constants; (4) preparation of review papers for Science, the American Journal of Physics, the Review of Particle Properties, and the Landolt-Bornstein Series.

ION KINETICS AND ENERGETICS DATA CENTER

Director: Sharon G. Lias
Center for Chemical Technology, NIST

The aim of the Data Center is to compile, evaluate, and disseminate data on ionization and appearance energies of ions from neutral precursor molecules, the enthalpies of formation of the resulting molecular and fragment ions, and on the rate constants for reaction of those ions with molecules.

A major publication of the data center, "Gas-phase Ion and Neutral Thermochemistry," by Sharon G. Lias (NIST), J. E. Bartmess (University of Tennessee), J. E. Liebman (University of Maryland Baltimore County Campus), J. L. Holmes (University of Ottawa), R. D. Levin (NIST), and W. G. Mallard (NIST) has been published in JPCRD. The publication gives evaluated enthalpies of formation of approximately 8000 ions (5600 cations and 2400 anions). Also, a computerized database is in preparation which contains the comprehensive background data used in this JPCRD publication.

The searchable database containing all these data was demonstrated at the American Chemical Society meeting and the American Society for Mass Spectrometry meeting, both in June. Suggestions for improvements in search schemes made by potential users at these demonstrations are now being implemented. The PC version of the database (Database 19) is scheduled for release in FY 1990.

Work on the update of the publication "Evaluated Gas Phase Basicities and Proton Affinities of Molecules: Heats of Formation of Protonated Molecules" has continued. The computer files have been reformatted preparatory to producing a PC version of the collection. The data are now being evaluated.

MOLECULAR SPECTRA DATA CENTER

Director: Frank J. Lovas
Center for Optical, Molecular, and Optical Physics, NIST

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, comparison, and derivation of a wide range of molecular properties. The molecular properties include energy levels, structures, molecular moments, and molecular constants needed to reproduce the spectra. One phase of the Center's work emphasizes microwave spectra of interstellar molecules for species identification, abundance determination, and molecular cloud properties such as temperature and velocity. The objective of this effort is to provide astronomers with a convenient source of molecular transitions previously identified in stellar and interstellar objects and to provide the most accurate measured or calculated transition frequencies available.

"Microwave Spectral Tables III. Hydrocarbons, CH to C₁₀H₁₀" by F. J. Lovas and R. D. Suenram is currently in press in the Journal of Physical and Chemical Reference Data. The manuscript includes about 130 tables of molecular constants and about 95 tables of spectral frequencies. This critical review contains all of the rotational spectral lines observed for 91 hydrocarbon molecules.

Work continues on the Microwave Spectral Tables IV, which treats organic species containing oxygen. The collection currently contains 171 species with empirical formulas CHO through C₇H₁₂O. Spectral data for 55 species (262 isotopic forms) have been coded for spectral fitting and table-generating programs.

Last year the Center collaborated on a survey of the Orion A molecular cloud in the 330 - 360 GHz frequency window. This project resulted in the observation of about 190 transitions from 37 species and 30 transitions from unknown molecular sources. These results have been submitted for publication (P. R. Jewell, J. M. Hollis, F. J. Lovas, and L. E. Snyder, *Astrophys. J. Suppl. Series*, 1989, in press).

Work is in progress on the next revision of the paper entitled "Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions - 1985 Revision" which was published in the January 1986 issue of the Journal of Physical and Chemical Reference Data. Completion of the revision is planned for late 1990. Since the 1986 publication, 18 new interstellar species have been identified, bringing the total number of identified molecules to 77. Many new transitions of the previously known species have also been reported, representing an approximate 20 percent increase in the amount of observational data.

MOLTEN SALTS DATA CENTER

Director: George J. Janz
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. Broadly, the aims encompass the development of standard reference data for molten salts physical properties from studies of the results in the open scientific literature, through critical evaluations and value judgments. Preparation of the results of these studies of BEST VALUES and PRODUCTS for users as authoritative compilations of BEST VALUES and DATA FOR COMPARISON PURPOSES are part of this program.

For the past year, SRD's effort has principally focused on critical data evaluations, extending the studies to newly reported systems and to database automation. Briefly, some of the activities include development of a

compilation of correlation equations for the critically evaluated properties, enhancement of the automation of the MSDC-RPI database, and evaluation of some corresponding states data correlations as predictive models for molten salts transport properties.

NATIONAL CENTER FOR THE THERMODYNAMIC DATA OF MINERALS

Director: John L. Haas (Retired in FY89)
Bruce S. Hemingway
U.S. Geological Survey
Reston, Virginia

The Center compiles, indexes, and evaluates data on the thermodynamic and thermophysical properties of minerals, their synthetic analogues, 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. The Center is also working with the CODATA Task Group on Chemical Thermodynamic Tables in their current work on iron and its compounds, especially in connection with the study of elemental iron and the oxides of iron.

NIST MASS SPECTROMETRY DATA CENTER

Director (Technical): Stephen E. Stein
Director (Administrative): Sharon G. Lias
Center for Chemical Technology, NIST

This is a new Data Center, created in October 1988, for the purpose of maintaining, updating, and improving the NIST/EPA/MSDC Mass Spectral Database. This computerized database of analytical mass spectra, originally developed 20 years ago by scientists at the EPA and NIH, has been distributed by the National Bureau of Standards since 1978. Currently NIST has primary responsibility for maintenance of the database. Thousands of copies of the database are in use in the data systems of commercial mass spectrometers, and in a PC version developed at NIST.

An update of the database was released to the public in December 1988. The database included 49,469 spectra, an increase of approximately 6,500 over the previous version. This was the largest increase in the size of the database in a decade. The December 1988 release also included, for the first time, structural information on about 85 percent of the compounds in the

database. Another update scheduled for early 1990 will incorporate an additional 5,000 spectra and structural information on all the compounds.

The release includes both a tape version, distributed mainly to instrument manufacturers who incorporate the database into the data systems of mass spectrometers, and a PC version for distribution to individual bench scientists. The PC version with search software was developed at NIST in 1987. The December 1988 PC version incorporated a number of new features, including several new search schemes and the capability for the user to add his own spectra to the collection, and search for matches, or compare the newly-added spectra to spectra already in the database.

A hard-copy version of an earlier edition of the database, The Wiley/NBS Registry of Mass Spectra (John Wiley & Sons, 1988), also appeared during FY89.

The initial examination by the NIST team of the database and the larger archive of spectra from which it is derived revealed that the spectra in the collection contained thousands of errors. An intensive effort was mounted to eliminate or correct erroneous spectra. About 65 percent of the errors were located before the December 1988 release. Until such time as the database is error-free, work will continue on cleaning up the archive of spectra from which the database is drawn. At the present time, every set of replicate spectra is being examined in order to select the best spectrum by observation; these selections were formerly made by a computer algorithm, which has proved to be inadequate since it often selected a poor spectrum over a good one. Many of the new spectra included in the updates were retrieved from the archival collection by correcting errors, or providing Chemical Abstracts Registry Numbers for the relevant compounds.

A high priority activity is the acquisition of new spectra to enlarge the database. The collection of chemicals in the Chemical Kinetics Division has been cross-checked against the contents of the database, and original spectra of all compounds not yet in the database are being determined in-house. Original spectra of widely-used commercially available compounds which are not now in the database are being provided under a new contract with Aldrich Chemical Company. Several existing collections of spectra have been located in mass spectrometry laboratories, and will be purchased for the database when funding becomes available. Under another ongoing contract, approximately 1,500 new spectra will be provided during the time period April 1, 1989-March 31, 1990.

PHASE DIAGRAMS FOR CERAMISTS DATA CENTER

Director: Stephen Freiman
Institute for Materials Science and Engineering, NIST

The purpose of the Phase Diagrams for Ceramists Data Center is to support the rapidly growing ceramics industry with evaluated ceramic phase diagrams. These diagrams present the relationship of processing conditions (e.g., T, P, composition) to thermodynamic equilibria of phases (solid, liquid, or gaseous). All inorganic, nonmetallic systems are covered, including oxides,

halides, sulfides, borides, carbides, nitrides, and semiconductors. These ceramic materials are used in a wide breadth of applications including structural, electronic, and optical, and they exhibit advantageous properties such as strength at high temperature, wear resistance, corrosion resistance, high and low dielectric constants, superconductivity, transmissivity, etc.

The long-range goals of the Data Center are threefold: (1) to develop a computerized database consisting of diagram graphics, keywords, critical evaluations, and the associated bibliography; (2) to expand the coverage to nonoxide systems and bring up to date the literature coverage, and (3) to disseminate the data to the user community in both computer and printed formats. To achieve these goals, NIST and the American Ceramic Society have established a cooperative program with additional support from industry and other Federal agencies.

The accomplishments of the cooperative program in the last year are succinctly summarized by the completion of Vol. 7 of Phase Diagrams for Ceramists. This volume contains more than 700 critical evaluations and 1000 individual diagrams and was produced entirely from the graphics, commentary, and bibliographic databases.

PHOTON AND CHARGED PARTICLE DATA CENTER

Director: Stephen M. Seltzer
Institute for Materials Science and Engineering, NIST

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.

A comprehensive review of the fluorescence yield for all elements, $Z = 1$ to 100, was prepared as a NIST Report entitled "Bibliography and Current Status of K, L, and Higher Shell Fluorescence Yields for Computation of Photon Energy-Absorption Coefficients," by J. H. Hubbell.

Electron and positron radiation yields needed for the calculation of bremsstrahlung factors in energy-absorption coefficients have been generated for some 28 materials of dosimetric interest and combined with the NIST database of photon cross sections (XGAM) to produce tables of the mass energy-transfer and mass-energy-absorption coefficients, from 10 keV to 100 MeV, for the 28 materials.

Tables of stopping powers (electronic, nuclear, and total), CSDA ranges, and projected ranges (penetration depths) have been prepared for protons with energies from 1 keV to 10 GeV and alpha particles with energies from 1 keV to 1 GeV in 73 materials of dosimetric interest.

The cross sections for elastic scattering of electrons have been accurately calculated using a partial-wave-expansion method for 11 kinetic energies from 1 keV to 1 MeV, for the elements $Z = 1$ to 100. The results have

been organized into a computer-readable database. Plans for FY 1990 include expansion of this database by (1) performing additional calculations for electrons at low energies where the cross sections have complicated structures and the present database is not sufficient for accurate interpolation; (2) doing the calculations for positrons at energies from 1 keV to 1 MeV; and (3) calculating the cross section at higher energies, from 1 MeV to 1 GeV, using a much more economical WKB method.

The EPSTAR computer code and database for the calculation, on a personal computer, of electron and positron stopping powers (collision, radiative, and total), CSDA ranges, density-effect corrections, and bremsstrahlung yields, at energies from 1 keV to 10 GeV and for any material, was completed and given to SRD for dissemination.

The cross sections for bremsstrahlung production by electrons with kinetic energies between 1 keV and 10 GeV and differential in emitted photon energy were converted into a computer-readable ASCII data file. The PC software to extract desired cross sections for any desired material and of energies is in preparation.

The completed critical review of fluorescence yields and other cross-section data provides sources for the input necessary in the calculation of the energy-absorption coefficients. In FY 1990 efforts will be directed toward numerically evaluating and combining the pertinent data and distributions for the calculation (ingredients include the shell-by-shell photoelectric cross sections and the corresponding fluorescence yields; the incoherent-scattering cross section and the resultant Compton electron energy spectrum; the pair and triplet production cross sections and the resultant energy spectra of electrons and positrons; the bremsstrahlung yield for electrons and positrons slowing down; and the in-flight annihilation of positrons). The development of the necessary codes for these calculations and the preparation of tables of results for all elements is expected to require a significant effort. The extension to compounds and mixtures may not be straightforward, because the secondary electron and positron factors are not accurately obtainable by simply adding the elemental results.

Plans for FY 1990 also include extension of our bibliography of experimental photon attenuation coefficients to include compounds. Such a source of information is necessary for thorough comparisons to test the limits of validity for mixture-rule results.

RADIATION CHEMISTRY DATA CENTER

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

The Center compiles, evaluates, and disseminates data on chemical reactions and photophysical processes initiated by the interaction of ionizing and photon radiation with matter. The activities particularly focus on

primary excited state processes of organic molecules in condensed phases and processes involving transient radicals in aqueous solution.

During FY 1989, critical data reviews were published on (1) rate constants for reactions of inorganic radicals in aqueous solution, (2) rate constants for quenching of excited states of metal complexes in fluid solution, and (3) one-electron reduction potentials involving radicals in aqueous solutions.

A critique of methods for determination of the molar absorptivity of transient species in solution and selection of preliminary standards was completed at the invitation of the IUPAC Photochemistry Commission.

RCDCbib, the bibliographic database, contains over 105,000 references; The Biweekly List of Papers on Radiation Chemistry and Photochemistry, produced from current additions to RCDCbib, is being distributed to over 500 persons. Online access is provided to RCDCbib and two numeric databases, RATES and TTAS.

Plans for FY 1990 include completion of the Handbook of Photochemistry, which will contain representative photochemical and photophysical data for a large number of organic molecules and other data relevant to the design of photochemical experiments. The article "Rate Constants for Reactions of Peroxyl Radicals in Fluid Solutions" will be published. A critical compilation of rate constants for reactions of transient intermediates from metal ions and metal complexes in aqueous solution, restricted to d-block transition metals, will be prepared. An update and reevaluation of kinetic data on the first excited singlet state of molecular oxygen in fluid solution is in progress.

THERMODYNAMIC RESEARCH CENTER

Director: Kenneth N. Marsh
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.

During the past year, the effort for SRD was directed towards the evaluation of the thermodynamic properties of organic nitrogen compounds; 1- and 2-butanamine, 2-methyl-1-propanamine, 2-methyl-2-propanamine, pyrrole, pyridine, and various substituted pyrroles and pyridines. Earlier work includes the study of eight primary amines. Properties being evaluated include condensed-phase properties, perfect gas properties and thermochemistry. The condensed-phase properties are primarily solid and liquid heat capacities and property changes at phase transitions. The perfect gas properties are thermal functions and the thermochemistry involves enthalpies

of formation (from combustion data) and equilibrium constants. Similar work is being completed for organic oxygen compounds.

Concurrent with this work, the data center has an ongoing program for abstracting information on the properties of organic compounds. During the past year, this information has been added to the TRC Source database.

TRIBOLOGY INFORMATION ACTIVITY

Director: Said Jahanmir
Institute for Materials Science and Engineering, NIST

A computerized tribology information system (ACTIS) is being developed to facilitate technology transfer to industry, to promote cross-disciplinary communication and to enhance the state-of-the art research. The system will consist of six elements: Numeric Data, Design Codes, Bibliographic, Newsletter, Research-in-Progress, and Product Literature databases. Work will be carried out in three phases. During Phase I, now ongoing, the system architecture will be established, and a prototype system that includes numeric data, design codes, and a newsletter will be developed.

This year, data evaluation projects for areas of tribology have been put into a numeric database that was designed and built by IMSE staff. A demonstration version of the entire system has been built and shown at several meetings.

ACTIS is sponsored by several government agencies and professional societies including NIST, DOE, NSF, and DOD as well as ASLE and ASME. Coordination of the activities and supervision of the work is done by the Tribology Group of the Ceramics Division at NIST.

PROJECTS

ANALYSIS OF TIME-DEPENDENT ELEVATED TEMPERATURE DATA

M. Prager
The Materials Properties Council
New York, New York
Source of Support: NSF, ASME, EPRI

This project is concerned with evaluating creep- and stress-rupture data for metallic alloys. The result will be a recommended practice for parametric analysis that can be used to validate elevated temperature of mechanical property data.

BINARY PHASE DIAGRAM EVALUATION

Copper Alloys

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

Vanadium Alloys

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

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

Iron Alloys

K. Okamoto
ASM International
Metals Park, Ohio
Source of Support: NSF

These evaluation projects are a major part of the National Institute of Standards and Technology (NIST)-ASM International (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.

CORROSION TEST SPOOL PROGRAM - COMPUTERIZED DATA RETRIEVAL SYSTEM

K. Money
LaQue Center for Corrosion Technology
Wrightsville Beach, North Carolina
Source of Support: NSF

As part of the NACE-NIST Corrosion Data Program, LaQue Center will provide data from over 7000 corrosion tests. These data have been collected over the last 40 years. Before sending to the Corrosion Data Center for detailed analysis and evaluation, LaQue is performing its own analysis including establishing the validity and completeness of the test description. These data represent one of the world's largest collections of corrosion rate data.

CREVICE CORROSION BEHAVIOR OF STAINLESS STEELS IN MARINE ENVIRONMENTS

K. Money
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 is being 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.

CRYSTALLOGRAPHIC DATA FOR ORGANIC MATERIALS

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

The Cambridge Crystallographic Data Centre has had a continuing collaboration with the NIST 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 NIST Crystal Data ID File, which is available for online use.

ENERGY LEVELS OF SMALL TRANSIENT MOLECULES

Marilyn E. Jacox
Center for Atomic, Molecular, and Optical Physics, NIST
Source of Support: NIST

The intention of this project is to provide critically evaluated data on the vibrational and electronic energy levels of small chemical reaction intermediates. These data are important to such diverse scientific applications as the determination of transient species in atmospheric pollution, the monitoring of plasmas in chemical vapor deposition and microcircuit etching systems, and the characterization of interstellar matter.

In an attempt to meet the need for these data, Dr. Jacox has published two compilations. The first of these (M. E. Jacox, J. Phys. Chem. Ref. Data 13, 945 (1984)) is concerned with the vibrational energy levels of small polyatomic (3 to 16 atoms) transient molecules and the second (M. E. Jacox, J. Phys. Chem. Ref. Data 17, 269 (1988)), with the electronic energy levels of transient molecules with from 3 to 6 atoms. Each of these publications contains data for approximately 500 molecules.

An effort to convert these data to computer-searchable files which can be distributed to the scientific community was started in mid-1989. All of the vibrational and electronic energy level data and literature references in the above two publications, plus more recent data for 266 additional molecules, have been included. As of 1 July 1989, these files contained energy level data for 1002 molecules, plus the corresponding energy levels for many of their fully deuterium-substituted counterparts. Menu development has proceeded with the help of the Data Systems Development Group of Standard Reference Data. Searches may be conducted over a user-specified range of frequencies or (for electronic energy levels) wavelengths. These searches can be limited by chemical composition or formula, by medium (e.g., gas phase, Ar matrix), or (for electronic energy levels) by whether the data were obtained in absorption or emission studies. All of the literature references for a given molecule or the literature references pertinent to individual energy levels can be displayed and printed. Menu refinement is in its final stages, and writing of the documentation is in progress. It is expected that the output will be ready for distribution in early 1990.

Also planned for FY 90 is a supplement to the earlier publications which will incorporate selective extensions to larger or somewhat less reactive molecules. Both vibrational and electronic data, as well as the principal rotational constants, will be included. It is estimated that this supplement will contain new or revised, critically evaluated data for 350 molecules. The supplement will be submitted to the Journal of Physical and Chemical Reference Data. In addition, a selective extension of the computerized database is planned.

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 has created a database of critically evaluated line energy for ESCA that was released for distribution in November 1989. Over 10,000 data records have been evaluated.

EVALUATION OF INORGANIC CRYSTALLOGRAPHIC DATA

JCPDS-International Centre for Diffraction Data
Swarthmore, Pennsylvania
Source of Support: NSF

The purpose of the project is to evaluate crystallographic data for inorganic substances and add them to the NIST Crystal Data File. The project makes heavy use of computer evaluation techniques developed at NIST and the JCPDS. The data come from both the University of Bonn and the JCPDS Powder Diffraction File.

FRACTURE TOUGHNESS OF HIGH STRENGTH ALUMINUM ALLOYS

J. G. Kaufman
MPD Network
Columbus, Ohio
Source of Support: NSF

Plane strain fracture toughness data for high strength aluminum alloys are critical to design and analysis in the aerospace industry. Building upon work done by the Aluminum Association Task Group on Fracture Toughness, this project will evaluate these data and build a database for distribution. Critical elements of the data source and quality will be addressed.

MATERIALS INFORMATION FOR SCIENCE AND TECHNOLOGY (MIST)
A Demonstration Project

R. P. Frosch
Rensselaer Polytechnic Institute
Troy, New York

W. L. Anderson
Engineering Algorithms, Inc.
Palo Alto, California

Sources of Support: NIST, DOE, DOD, National Laboratories

The MIST demonstration project is a joint effort between NIST and DOE to build a prototype materials data system. During the past three years, two phases have been completed including development of a flexible, extensible database schema and its implementation on the Spires DBMS at Stanford University. The system was demonstrated in May 1987 and is now operational to a limited user community. A major reimplementaion was completed in 1988.

The major goals of the project are twofold:

1. To demonstrate that a comprehensive materials data system can be built
2. To provide a solid foundation for building operational systems in the future.

Work is being done in close cooperation with the National Materials Property Data Network.

POLYMER-POLYMER MISCIBILITY DATA

S. Krause
Rensselaer Polytechnic Institute
Troy, New York
Source of Support: NSF

Polymer-polymer miscibility data are important in polymer processing. The result of this project will be a database of evaluated miscibility data. The first year will cover compatible polymers; the second year, immiscible mixtures.

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 is critically examining 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 SPUTTERING YIELD PROJECT

Joseph Fine
Center for Atomic, Molecular, and Optical Physics, NIST
Sources of Support: DOE and NIST

Sputtering techniques for depth profile are used with 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 is preparing a compilation of evaluated sputtering yield data for several ion species and energies for targets of pure elements.

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 has critically examined all LEED data and assessed their quality. It covered elemental surfaces and the compound ionics and semiconductors. An article was published in JPCRD in 1987. A database is now being built.

COVERAGE DATA FOR MOLECULAR ADSORPTION ON TRANSITION METALS

T. Gustafsson
Rutgers University
Piscataway, New Jersey
Source of Support: NSF

This is a new project to provide a critical compilation of data on the absolute coverage of adsorbed molecules or well-characterized transition metal surfaces.

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.

CHEMICAL THERMODYNAMIC PROPERTIES OF POLYCYCLIC AROMATIC HYDROCARBONS

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

Tables of standard chemical thermodynamic properties of polycyclic aromatic hydrocarbons are being calculated. These tables for the ideal gas phase cover 298 K to 3000 K because of the importance of these data in understanding soot formation in flames, the high temperature vaporization of graphite, and astrophysical calculations. As the number of 6-member rings increases, the number of different structures with the same number of carbon atoms increases, and the numbers of isomers increase. Therefore, isomer group thermodynamic properties and distributions within isomer groups are being calculated. There is an infinite number of "homologous" series of polycyclic aromatic hydrocarbons, but studying the first half dozen series and the first members for a larger number of series should make it possible to generalize the thermodynamic properties of all polycyclic aromatic isomer groups. Recent work has focused on the completion of the linear regression of pyrene series and the naphthopyrene series of polycyclic aromatic hydrocarbons.

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 scientifically based and validated representative equations for the thermodynamic and transport properties of fluids as a function of pressure and temperature. The equations are applied to evaluate and synthesize available experimental and theoretical information for the thermophysical properties of fluids in a form suitable for inclusion in data banks.

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

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

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, regulation, standardization, or codification in some aspect of pure or applied chemistry. There are 10 international cooperating centers for this work: France (1), FRG (3), Japan (1), Norway (1), UK (2), USA (2).

NEW METHODS FOR THE DETERMINATION OF AN EQUATION OF STATE FOR MIXTURES OF NITROGEN, ARGON AND OXYGEN AND OF AIR

R. T. Jacobsen
University of Idaho
Moscow, Idaho
Source of Support: NSF

The objective of this research project is to develop new equations of state for binary and ternary mixtures of the N_2 -Ar- O_2 system that are accurate for any mixture composition. The resulting property formulations and property tables will be used in commercial applications including aerospace flight and separation and liquefaction of air. The relatively large quantity of available experimental data for the N_2 -Ar- O_2 system provides a unique situation for the study of methods of correlating mixture data.

This project is closely coordinated with work on air at NIST Boulder and the techniques of the project are being considered for possible use in studies of liquefied natural gas and other hydrocarbon mixtures.

DIPPR DATA PROJECTS

AIChE

New York, New York

Sources of Support: NIST, 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 NIST and AIChE, the parent organization of DIPPR, DIPPR and NIST will cooperate in a variety of ways in the production of critically evaluated data for industry.

Currently, NIST is involved directly with two DIPPR activities: the critical evaluation of physical property data of pure compounds and the evaluation of data on the thermodynamic properties of aqueous solutions over a range of temperatures.

CRITICAL TABLES OF OBSERVED PROPERTIES OF LIQUID HELIUM, ^4He

R. J. Donnelly

University of Oregon

Eugene, Oregon

Source of Support: NSF

Accurate formulations for the observed properties of liquid helium at the saturated vapor pressure will be developed and published in the form of printed tables, and in the form of floppy disks.

Quantities under study include the velocities of first, second, third, and fourth sound, entropy, specific heat, thermal conductivity, positive and negative ion mobilities, mutual friction coefficients B and B' , the dispersion relationship, the vapor pressure scale T58, and the condensate fraction.

CRITICAL EVALUATION OF HIGH-TEMPERATURE KINETIC DATA

N. Cohen

Aerospace Corporation

Los Angeles, California

Source of Support: NSF

The aim of this project is the critical evaluation of high-temperature chemical kinetic data in three areas of combustion- and propulsion-related chemistry: (1) the reactions of H atoms with alkanes; (2) the reactions of O, H, and OH with ammonia, hydrazine, and other $\text{N}(x)\text{H}(y)$ species; and (3) high-temperature nitrogen-oxygen chemistry, including neutral, ionized, and

electronically excited species. The output of this activity is a series of data sheets, in a format previously developed and utilized, that will be submitted for publication to JPCRD.

A CENTRALIZED DATABASE FOR THERMODYNAMIC DATA OF LIPID MESOMORPHIC PHASE TRANSITIONS AND MISCIBILITY

Martin Caffrey
Department of Chemistry
The Ohio State University
Columbus, Ohio
Source of Support: NSF

The systematic study of the mesomorphic phase properties of synthetic and biologically-derived lipids began some 20 years ago. In the past decade, interest in this area has grown enormously. As a result, there exists a wealth of information on lipid phase behavior but, unfortunately, the data are scattered throughout the literature in a variety of journals, books, and proceedings, both foreign and domestic. This project involved the compilation and evaluation of these data with a view to providing ready access to the data and to the appropriate literature. The compiled evaluated data will be gathered into a single, continuously updated computer program. Hard copies of the data will also be available on request.

The compilation is being prepared in two parts. The first is a tabulation of all known and evaluated mesomorphic and polymorphic phase transition temperatures and enthalpies for synthetic and biologically-derived lipids in the dry and in the partially and fully hydrated states. The second part concerns the miscibility properties of the lipids. In this part, the data will be graphically presented in the form of evaluated isobaric and isothermal phase diagrams.

ESTABLISHING CONSISTENT THERMODYNAMIC DATA ON VAPORIZATION EQUILIBRIA IN ONE COMPONENT SYSTEM

Vladimir Majer
Department of Chemistry and Biochemistry
University of Delaware
Newark, Delaware
Source of Support: NSF

Vapor pressure data are abundant and accurate near the normal boiling point while they are scarce and unreliable in the low-pressure range. Data on thermal properties (enthalpy of vaporization and difference in the heat capacities of an ideal gas and the liquid) are available, however, at temperatures far below the normal boiling point. All three properties are related by exact thermodynamic relationships and can be correlated simultaneously. This procedure can be used in the evaluation of thermodynamic data on vaporization equilibria as a rigorous consistency test and for producing recommended data sets. When a suitable correlation equation is selected, a single set of

parameters permits generation of consistent data for several properties between the triple and normal boiling points. The procedure is especially useful for calculating vapor pressures and/or enthalpies of vaporization far below the normal boiling point. The application of this method for establishing the reference data for the selected groups of compounds (alkanols and n-alkanes) is proposed. A universal correlation program will also be produced that will serve as part of the software of a data bank containing thermodynamic properties. In combination with the group contribution methods for estimation of thermal properties, the principle of simultaneous correlation can serve as a base in the formulation of a new approach to the estimation of vapor pressures of high boiling compounds.

PROPERTIES OF POLAR FLUIDS

Richard F. Kayser
Center of Chemical Technology, NIST
Source of Support: NIST

Major activities in this area include modeling of high-temperature aqueous solutions, determination of the solubility of gases and Henry's constants, reformulation of the refractive index of water and steam, examination of the molecular dynamics of hydrogen bonding, investigation of the hydrogen bonding in aqueous solutions, compilation of water and steam data, development of a computer package on refrigerant properties, and participation in IAPS activities.

APPLICATION OF EXPERT SYSTEMS TO CRITICAL EVALUATION OF THERMOPHYSICAL PROPERTY DATA

J. C. Holste and K. R. Hall
Texas A & M Research Foundation
College Station, Texas
Source of Support: NSF

This activity involves the design and development of an expert system to assist compilers of thermodynamic data in critical aspects of the evaluation and selection process. The expert system will be interfaced with a large computerized database of numerical experimental values of thermodynamic properties maintained by the Thermodynamics Research Center. An expert system is a computer program that draws on the organized expertise of one or more human experts. Their advice is coded as rules which, along with a knowledge base, constitute the expert system building program. By taking actions specified by the rules, the computer simulates the behavior expected of human experts when solving the same critical data evaluation problem. The system itself also provides a precise record of the process leading to particular selections. By relieving compilers of much of the tedious and routine aspects of their work, it will be possible to carry out frequent and timely analyses of the current state of thermodynamic knowledge in particular areas with greater efficiency and at reduced cost. The process of developing and testing of the expert system will also lead to a better formulation and definition of

the evaluation and selection procedures. The system itself will serve as a precise record of the processes leading to particular selections.

THERMODYNAMIC PROPERTIES OF ALKENES

Dr. William V. Steele
National Institute for Petroleum and Energy Research
IIT Research Institute
P.O. Box 2128
Bartlesville, Oklahoma 74005
Source of Support: NSF

The purpose of the work is to upgrade the state of thermodynamic data on alkenes so that this functional class of organic compounds will be as well-defined as the alkanes. The objectives of the project are to: collect and assess the available thermodynamic and thermophysical data for C₃ alkenes and alkenes with greater carbon numbers, prepare a comprehensive report on the available data assessing reliability, precision, and accuracy, determine and identify gaps in the data where a particular thermodynamic measurement is missing, and derive a comprehensive set of group-additivity parameters to permit estimation of the thermodynamic properties for alkene where experimental data are poor or unavailable. A final report on the work of the project will result in a publication for JPCRD.

CRITICAL STABILITY CONSTANTS AND RELATED THERMODYNAMIC CONSTANTS OF METAL COMPLEXES

Dr. Arthur E. Martell
Department of Chemistry
Texas A & M University
College Station, Texas 77843
Source of Support: NIST

A database is in preparation consisting of critical stability constants of metal complexes in aqueous solution and related critical equilibrium constants such as hydrolysis and protonation constants of the complexes, and protonation constants of the complexing agents. In addition to the standard Gibbs energy values, provided in the form of equilibrium constants, the corresponding standard enthalpy values will be evaluated, when available. Stability constants and other thermodynamic constants for aqueous solutions at all temperatures and all ionic strengths of supporting electrolytes will be part of the database. Similarly, solubility product constants (K_{sp}) for solid-solution equilibria of metal hydroxides and other frequently encountered metal precipitates will be evaluated and included in the database.

THERMOCHEMICAL DATABASE FOR THE ELEMENTS

C. B. Alcock
Department of Materials Science and Engineering
University of Notre Dame
Notre Dame, Indiana 46556
Source of Support: NIST

The purpose of the project is to review the experimental thermochemical data for the Group IIA elements (beryllium, magnesium, calcium, strontium, barium, and radium) and to examine the structure of a computerized database currently in use at the University of Notre Dame which will accommodate the thermochemical information. The prime deliverable of the work is a set of recommended thermochemical values for the designated elements and the background (bibliographic and evaluational) information used in the derivation of the recommended values.

NIST CHEMICAL ABSTRACTS SERVICE REGISTRY NUMBER FILE

K. N. Marsh, B. Gammon, and R. C. Wilhoit
Department of Chemistry
Texas A & M University
College Station, Texas 77843
Source of Support: NIST

The purpose of this project is to develop a computer program and searchable file containing Chemical Abstracts Service (CAS) Registry Numbers suitable for searching and updating on a mainframe or microcomputer. The program can be searched for compound name, formula, or CAS Registry Number. At the present time, about 6000 organic compounds can be searched in the current database. Plans for FY 1990 include adding a large number of inorganic compounds to the database.

DETERMINATION OF EQUATIONS OF STATE FOR REFRIGERANTS AND REFRIGERANT MIXTURES

Professor R. T. Jacobsen
Center for Applied Thermodynamic Studies
University of Idaho
Moscow, Idaho
Source of Support: NSF

The project objective is to develop new reference equations of state for several halocarbon refrigerants which do not contribute to atmospheric ozone depletion. The alternative refrigerants are R-22, R-123, R-134a, R-141b, and R-152a. The use of these fluids in future commercial applications will depend on the existence of accurate equations of state. Recent data reported on compressibilities, heat capacities, and velocities of sound will be added to

the database used in the development of the new equations of state for these refrigerants. Predicted property values based on extended corresponding states methods will be used where experimental data are not available.

This work is being coordinated by SRD with similar and related projects at NIST Gaithersburg, NIST Boulder, and the University of North Dakota.

DETERMINATION OF ANCILLARY FUNCTIONS FOR THE REPRESENTATION OF THE VAPOR-LIQUID COEXISTENCE CURVES OF SEVERAL REFRIGERANTS

S. G. Penoncello
Center for Applied Thermodynamic Studies
University of North Dakota
Box 8214
Grand Forks, North Dakota 58202
Source of Support: NSF

The project objective is to develop reference equations for the vapor pressure, saturated liquid density, and saturated vapor density for the following alternative refrigerants R-22, R-123, R-134a, R-141b, and R-152a because they do not contribute to the ozone depletion of our atmosphere. New methods of coexistence property prediction will be developed where experimental data are unavailable. One fluid and multi-fluid corresponding states models will be investigated. Particular attention will be given to saturated vapor density values. The accuracy of the resulting equations will be confirmed by comparing the calculated properties with the experimental and predicted values.

This work is being coordinated by SRD with similar and related projects at NIST Gaithersburg, NIST Boulder, and the University of Idaho.

CRITICAL EVALUATION AND COMPILATION OF THERMODYNAMIC AND VAPORIZATION DATA FOR METAL SULFIDES

Paul W. Gilles
Department of Chemistry
University of Kansas
Lawrence, Kansas
Source of Support: NSF

The purpose of the project is to prepare a critical compilation of the thermodynamic and vaporization properties of sulfides of sodium, rubidium, and cesium for the gas, liquid, and solid phases. The data to be evaluated will include: calorimetric measurements from low temperatures to room temperature, high-temperature (700-2500 K) vaporization measurements, solid-state EMF measurements, solubility measurements, high temperature equilibrium measurements in systems containing flowing reactive gases, Knudsen cell mass spectrometric measurements of gas phase systems, and other related spectroscopic measurements. Thermodynamic and vaporization data are of importance to the metallurgical industries, in processes which require corrosion control,

recovery of chemicals destined for waste disposal, operation of electrochemical systems, and in the monitoring and regulation of sulfur compounds in pollution control.

COMPUTER PROGRAM ON THERMOPHYSICAL PROPERTIES OF FLUIDS

William A. Wakeham
IUPAC Thermodynamic Tables Project Centre
Imperial College of Science, Technology, and Medicine
London SW7 2BY England
Source of Support: NSF

The project objective is to provide an interactive program and computerized databases containing complete equations of state and transport properties for pure fluids. The programs and databases are founded upon IUPAC publications prepared at the IUPAC Thermodynamic Tables Project Centre. Recent volumes published deal with thermodynamic tables of the fluid state for oxygen (volume 9) and ethylene (volume 10). The volume on fluorine (volume 11) will be available soon while volumes on sulfur hexafluoride (volume 12) and methanol (volume 13) are in preparation.

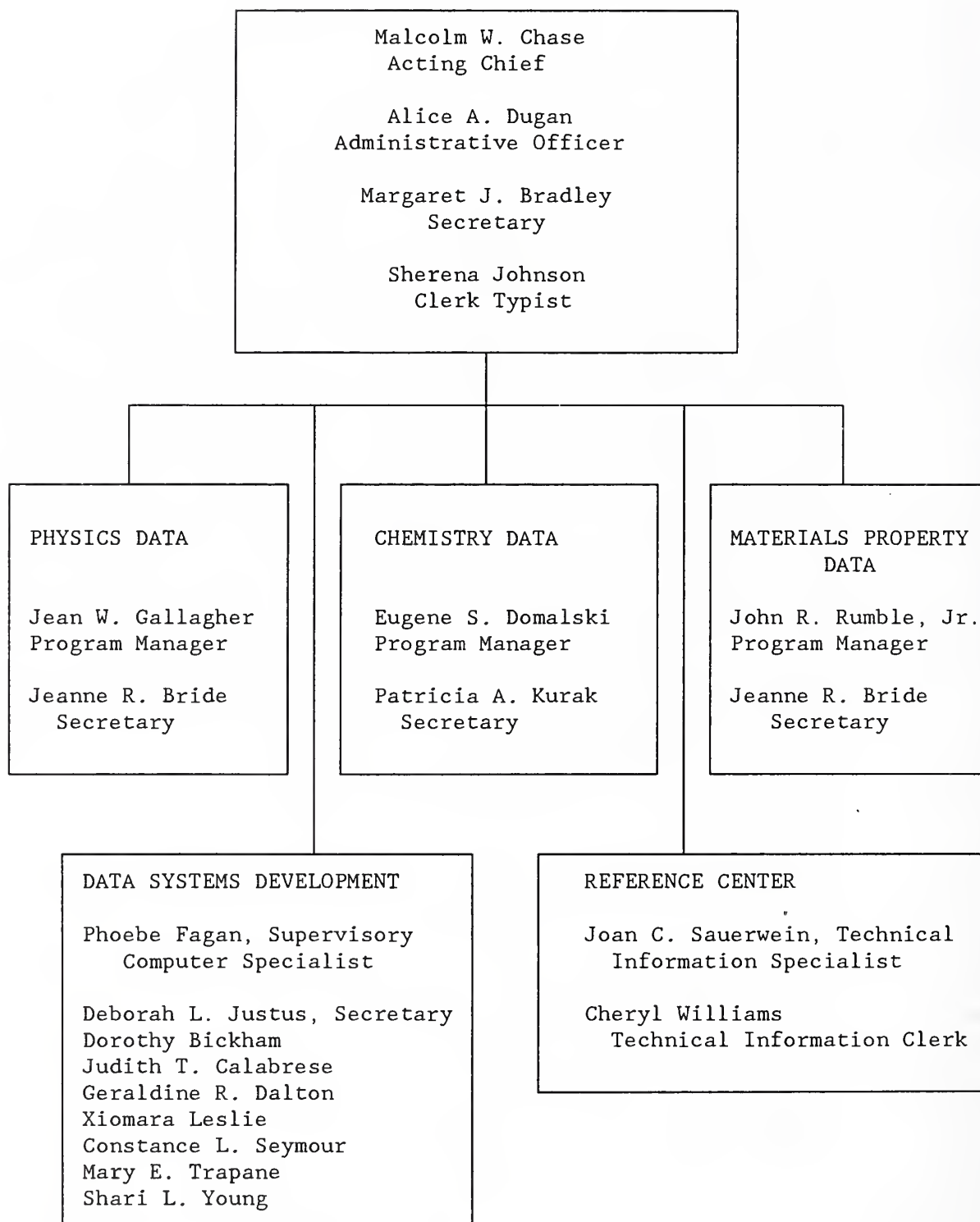
LIST OF ACRONYMS AND ABBREVIATIONS

AAAS	American Association for the Advancement of Science
AAPM	American Association of Physicists in Medicine (AIP)
ACerS	American Ceramic Society
ACS	American Chemical Society
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 International
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, NIST
CAD	Computer-Aided Design
CAM	Computer-Aided Manufacturing
CAMOP	Center for Atomic, Molecular, and Optical Physics
CAS	Chemical Abstracts Service
CCE	Center for Chemical Engineering, NEL, NIST
CCT	Center for Chemical Technology, NML, NIST
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, NIST
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)
JANNAF	Joint Army, Navy, NASA, Air Force
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, NIST-University of Colorado
LEED	Low Energy Electron Diffraction
MPC	Materials Properties Council
MSDC	Mass Spectral Data Centre (UK)
NACE	National Association of Corrosion Engineers
NAS	National Academy of Sciences
NAVLAP	National Voluntary Laboratory Accreditation Program
NIST	National Institute of Standards and Technology
NCI	National Cancer Institute
NEL	National Engineering Laboratory, NIST
NIH	National Institutes of Health
NLM	National Library of Medicine
NML	National Measurement Laboratory, NIST
NMPDN	National Materials Property Data Network
NMR	Nuclear Magnetic Resonance
NRC	National Research Council
NSF	National Science Foundation
NSRDS	National Standard Reference Data System
NTIS	National Technical Information Service
OA	Other Agency (Funding)
OMS	Office of Measurement Services, NML, NIST
ONR	Office of Naval Research
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 Materials
STRS	Scientific and Technical Research and Services (appropriated NIST funds)
UNESCO	United Nations Educational, Scientific, and Cultural Organization
USGS	United States Geological Survey

December 18, 1989

STANDARD REFERENCE DATA



STAFF OF STANDARD REFERENCE DATA

Acting Chief - Dr. Malcolm W. Chase
Secretary, Mrs. Margaret J. Bradley
Clerk Typist, Sherena Johnson
Telephone: (301) 975-2200

Administrative Officer - Ms. Alice A. Dugan
Telephone: (301) 975-2202

Fiscal and budgetary matters; contracting; procurement; personnel.

Program Manager - Dr. Jean W. Gallagher
Secretary, Mrs. Jeanne R. Bride
Telephone: (301) 975-2204

Management of Physics Data Program - atomic, molecular, and nuclear properties data.

Program Manager - Dr. Eugene S. Domalski
Secretary, Mrs. Patricia A. Kurak
Telephone: (301) 975-2205

Management of Chemistry Data Program - kinetic, thermochemical, and thermophysical data.

Program Manager - Dr. John R. Rumble, Jr.
Secretary, Mrs. Jeanne R. Bride
Telephone: (301) 975-2203

Management of Materials Property Data Program - mechanical properties, corrosion, phase diagrams.

Reference Center - Mrs. Joan C. Sauerwein
Assistant, Cheryl Williams
Telephone: (301) 975-2208

Distribution of databases; coordination of SRD publication process; response to data inquiries from the public; maintenance of NSRDS collection of main NIST Library and SRD Reference Center holdings.

Guest Scientist - Dr. Lewis H. Gevantman
Telephone: (301) 975-2210

As Secretary of IUPAC Commission on Solubility Data, plans and monitors progress of work of the Commission and looks for opportunities for joint data activities with NSRDS data centers.

Guest Scientist - Dr. David R. Lide
Telephone: (301) 975-2201

Editor, Journal of Physical and Chemical Reference Data. As President of CODATA and Chairman of the IUPAC Committee on Chemical Databases, oversees the work of these two international groups, including cooperative projects in which NIST scientists participate.

Guest Scientist - Dr. Howard J. White, Jr.
Telephone: (301) 975-3190

Monitors the activities of DIPPR, the International Association for the Properties of Steam, and related organizations in the preparation of numerical databases and consults on such activities of importance to NIST or involving NIST participation.

Data Systems Development Group
Phoebe Fagan
Secretary, Deborah Justus
Telephone: (301) 975-2213

Oversight of SRD activities related to automation, database development and dissemination; System manager and consultant for SRD Computer Facilities.

Mrs. Dorothy Bickham
Telephone: (301) 975-2524

Software development and application for data automation and dissemination; database design and implementation.

Mrs. Judith T. Calabrese
Telephone: (301) 975-2215

Oversight of the Bedford Composition system including system management and consulting; programming for system control, data conversion, and computer typesetting; coordination of user interfaces to the composition system.

Mrs. Geraldine R. Dalton
Telephone: (301) 975-2214

Development of software for data automation; design of database systems; automation of data center activities; preparation of databases for distribution.

Mrs. Constance L. Seymour
Telephone: (301) 975-2217

Publication control of NSRDS manuscripts for computer typesetting; processing and pagination of files received from outside data centers through composition system.

Miss Mary E. Trapane
Telephone: (301) 975-2219

Programming for data automation and dissemination; processing of files for typesetting; preparation of graphics for publications.

Miss Shari L. Young
Telephone: (301) 975-2212

Development and utilization of software for data automation and dissemination; major assistance in SRD Computer Facilities support.

Miss Xiomara Leslie
Telephone: (301)975-3207

Coop student in chemistry at the University of Maryland; data entry and graphical evaluation of published inorganic thermodynamic data.

PUBLICATIONS BY SRD STAFF

"Numerical Databases in Chemical Thermodynamics at the National Institute of Standards and Technology," Malcolm W. Chase, J. Res. Natl. Inst. Stand. Technol. 94, 21-24 (1989).

"Thermodynamic Properties of the Alkaline Earth Hydroxides: A JANAF Case History," Malcolm W. Chase and Rhoda Levin, High Temperature Science, In press, (1989).

"Energy of Combustion of Triphenyl Phosphate," D. R. Kirklin and S. Domalski, J. Chem. Thermodynam. 21, 449-456 (1989).

"Bomb Calorimetric and NMR Studies on Crystalline Hexaglycine," J. C. Colbert, E. S. Domalski, B. Coxon, and D. L. VanderHart, Thermochemica Acta 153, 123-141 (1989).

"Estimation of the Thermodynamic Properties for Organic Compounds at 298.15 K. Part I. Estimation Algorithm and Database for Hydrocarbon Compounds," E. S. Domalski and E. D. Hearing, NIST Technical Note (accepted) (1989).

"Enthalpy of Combustion of Dimethyl-1,4-cubane dicarboxylate," D. R. Kirklin and E. S. Domalski, J. Chem. Thermodynam. 21, (in review) (1989).

"FORTRAN from RTE to HP-UX," Phoebe Fagan, TC Interface Magazine, July (1989).

"Measurements of Electron Impact Optical Excitation Functions," D. W. O. Heddle and Jean W. Gallagher, Rev. Mod. Phys. 61, 221-278 (1989).

"Multiphoton Bibliography 1983-1986," S. J. Smith, J. H. Eberly, J. W. Gallagher, NBS LP-92, Suppl. 5, June 1989.

"Numerical Databases for Chemists: Present and Future," David R. Lide, Proceedings of the 1989 International Chemical Information Conference, Elsevier Publishing Co. (1989).

"Computerization and Networking of Materials Data Bases," J. Glazman and J. Rumble, Jr., Editors, ASTM Special Publication 1017 (ASTM, Philadelphia, PA 1989).

"Socioeconomic Barriers in Computerizing Materials Data," J. Rumble, Jr., in "Computerization and Networking of Materials Data Bases," J. Glazman and J. Rumble, Jr., Editors, ASTM Special Publication 1017 (ASTM, Philadelphia, PA, 1989).

"Making Materials Database Standards International," J. Rumble, Jr., ASTM Standardization News, 17, 32-36 (1989).

"Computerized Materials Property Data Systems," J. Rumble, Jr., D. Anderson, and J. G. Kaufman, Sea Technology, June (1989).

"Standard Reference Data Publications 1987-1989," Joan C. Sauerwein, NIST Special Publication 708, Supplement 2, December (1989).

TALKS AND PRESENTATIONS BY SRD STAFF

Malcolm W. Chase

"The Standard Reference Data Program and the JANAF Thermochemical Tables," NASA Lewis Research Center, Cleveland, OH, and General Electric Lighting, Metals Park, OH, August 22-23, 1989.

"The Standard Reference Data Program," Numerical Data Advisory Board Mtg., Washington, DC, September 21, 1989.

"PC Demonstration of Thermodynamic Databases," Sixth International Conference on High Temperatures - Chemistry of Inorganic Materials, NIST, Gaithersburg, MD, April 3-7, 1989.

"Thermodynamic Properties of the Alkaline Earth Hydroxides: A JANAF Case History," Sixth International Conference on High Temperatures - Chemistry of Inorganic Materials, NIST, Gaithersburg, MD, April 3-7, 1989.

Eugene S. Domalski

"Thermochemistry of High-Energy Reactions," U.S. Army/CRDEC Conference on Chemical Defense, Aberdeen Proving Ground, MD, November 15, 1989.

Jean W. Gallagher

"Atomic and Molecular Data Needed for Astronomy and Astrophysics," CODATA, Karlsruhe, FRG, September 26 - 28, 1988.

NIST - Ohio, Pennsylvania, West Virginia State Technology Extension Agents Seminar, Wheeling, W. Virginia, January 23-25, 1989.

"The Standard Reference Data Program," New York University - Physics Department Seminar - February 27, 1989.

"Atomic Physics Data Programs at the National Institute of Standards and Technology," American Physical Society, Division of Atomic, Molecular, and Optical Physics Meeting, Windsor, Ontario, Canada, May 1989.

"Atomic Physics Data Programs at the National Institute of Standards and Technology," Sixteenth International Conference on the Physics of Electronic and Atomic Collisions, New York, New York, July 26 - August 1, 1989.

"Databases of Atomic Collisions Cross Sections," Sixteenth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies, Chicago, Illinois, October 1-6, 1989.

John R. Rumble

"Materials Database Standards," ASTM Workshop on Numbering Systems for Nonmetals, Philadelphia, PA, February 1989.

"Computer Access to Technical Information: What is the Future," Syracuse University, Syracuse, NY, March 1989.

"User Interfaces for Scientific Databases," NIST, Gaithersburg, MD, March 1989.

"NIST X-Ray Photoelectron Spectroscopy Database," ASTM Committee E42 Technical Update Meeting, Cleveland, OH, May 1989.

"ASTM Activities on Materials Data Exchange Formats," Rolls-Royce Workshop on Materials Data Exchange, Derby, U.K., September 1989.

"The Uses of Materials Information," ALCOA Laboratories Technical Symposium, Nemacon Woodlands, PA, October 1989.

"International Standardization for Materials Databases," ASM Metals Week, Indianapolis, IN, October 1989.

"NIST X-Ray Photoelectron Spectroscopy Database," American Vacuum Society, Boston, MA, October 1989.

"Standards for Materials Databases - ASTM Committee E49," Second International Symposium on Computerization of Materials Property Databases, Lake Buena Vista, FL, November 1989.

"Search Strategies for Materials Databases - Approaches for Large Databases and Systems," Second International Symposium on Computerization of Materials Property Databases, Lake Buena Vista, FL, November 1989.

"Numeric Database for Tribology: Format and Application Issues," Second International Symposium on Computerization of Materials Property Databases, Lake Buena Vista, FL, November 1989.

EXHIBITS BY SRD STAFF

<u>NAME</u>	<u>LOCATION</u>	<u>DATES</u>
Pittsburgh	Atlanta	6-10 March 1989
Petro Expo '89	Houston	4-6 April 1989
National ACS Meeting	Dallas	9-12 April 1989
CLEO	Baltimore	25-27 April 1989
National APS Meeting	Baltimore	1-4 May 1989
Lake Forest	Gaithersburg	1-22, May 1989
Health Physics Society	Albuquerque	26-28 June 1989
EnvirACS	Washington, DC	25 - 27 July 1989
Materials, Services, & Applications Expo.	Indianapolis	2-4 October 1989

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Dorothy Bickham

Baltimore-Washington, DC, HP UNIX Users Group

Judith T. Calabrese

Bedford Composition System Users Group
TypeX, GraphX, and ArtX trade shows

Malcolm W. Chase

CODATA Task Group on Chemical Thermodynamic Tables (Chairman)

Engineering Sciences Data Unit Ltd., Physical Data and Reaction Kinetics
Committee (Corresponding Member)

ASTM E27 Hazard Potential of Chemicals (Chairman)

ASTM E49 Computerization of Material Property Data

Journal of Physical and Chemical Reference Data (Editorial Board & Management
Board)

ACS Task Force on Numerical Scientific Data

Design Institute for Physical Properties Data (DIPPR) (AIChE)

Administrative Committee

Technical Committee (non-voting)

Liaison Committee

Data Compilation Project Advisory Committee

Electrolyte Data Project Advisory Committee

Geraldine R. Dalton

Baltimore-Washington, DC, HP UNIX Users Group (Newsletter Editor)

Eugene S. Domalski

American Chemical Society

American Society of Mechanical Engineers (Associate Member)

American Society of Mechanical Engineers - Research on Industrial and
Municipal Wastes

ASTM E27 Hazard Potential of Chemicals

ASTM E38 Research Recovery

IUPAC Subcommittee on Thermodynamic Data of the Commission I.2 on Thermodynamics (Secretary)

Design Institute for Physical Properties Data (DIPPR) (AIChE)
Technical Executive Committee
Data Compilation Project Advisory Committee
Electrolyte Data Project Advisory Committee
Evaluated Data on Mixtures Advisory Committee

Phoebe Fagan

User Committee for Scientific Computing, NIST

Baltimore-Washington, DC, Hewlett Packard UNIX Users Group (Chairman)

SIGUNIX, Interex, (Survey Chairman)

Jean Gallagher

American Physical Society Committee on Numerical Databases

Joint Committee on Atomic and Molecular Physical Data (JCAMP)

"Workshop on Atomic Physics Databases" - NIST, 1-3 March 1989
Organizing Committee

Sixth International Swarm Seminar, Glen Cove, Long Island, New York,
2 - 5 August 1989, Organizing Committee

David R. Lide, Jr.

American Institute of Physics (AIP Publication Board)

Committee on Nomenclature, ACS

Journal of Physical and Chemical Reference Data (Editor)

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

Committee on Chemical Databases, IUPAC (Chairman)

Advisory Council, Engineering Information, Inc.

Advisory Committee, Particle Data Center, Lawrence Berkeley Laboratory

International Council for Scientific and Technical Information (Executive
Committee)

ACS Task Force on Numerical Scientific Data (Chairman)

Editorial Board, Journal of Chemical Information and Computer Science

U. S. Advisory Committee for the International Council of Scientific Unions

John Rumble

ASTM E-49 Computerized Materials Data (Chairman)

ISO/TC184/SC4/WG1 Standard for the Exchange of Product Data, Materials Committee (Chairman)

ASTM Committee on Publications

ACTIS, Inc. - Board of Directors

National Materials Property Data Network - Technical Advisory Group

NIST/International Centre for Diffraction Cooperative Program on Crystal Data Management Board

VAMAS Technical Working Area 10 on Materials Databanks (Co-Chairman)

Alloy Phase Diagram International Commission (NIST Representative)

ASM International - Metals Information Committee

ASTM Committee E-42 Surface Analysis

Second International Symposium on Computerization and Networking of Materials Databases, Orlando, FL, December 1989 (Organizing Committee)

ALCOA Laboratories Technical Symposium, "Opportunities for Computer Science to Advance Materials Science," Nemacon Woodlands, PA, October 1989 (Organizing Committee)

Constance L. Seymour

Bedford Composition System Users Group

Mary Trapane

Baltimore-Washington, DC, HP UNIX Users Group
SIGUNIX of Hewlett Packard International Technical Users

Howard J. White

International Association for Properties of Steam (Executive Secretary)

ASME Research and Technology Committee on Water and Steam in Thermal Power Systems (Member)

Design Institute for Physical Properties Data (DIPPR) (AIChE) (Member)
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Data Compilation Project Advisory Committee
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Journal of Chemical and Engineering Data (Editorial Advisory Board)

Shari L. Young

Baltimore-Washington, DC HP UNIX Users Group



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:

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

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

June 27, House concurred in Senate
amendments.

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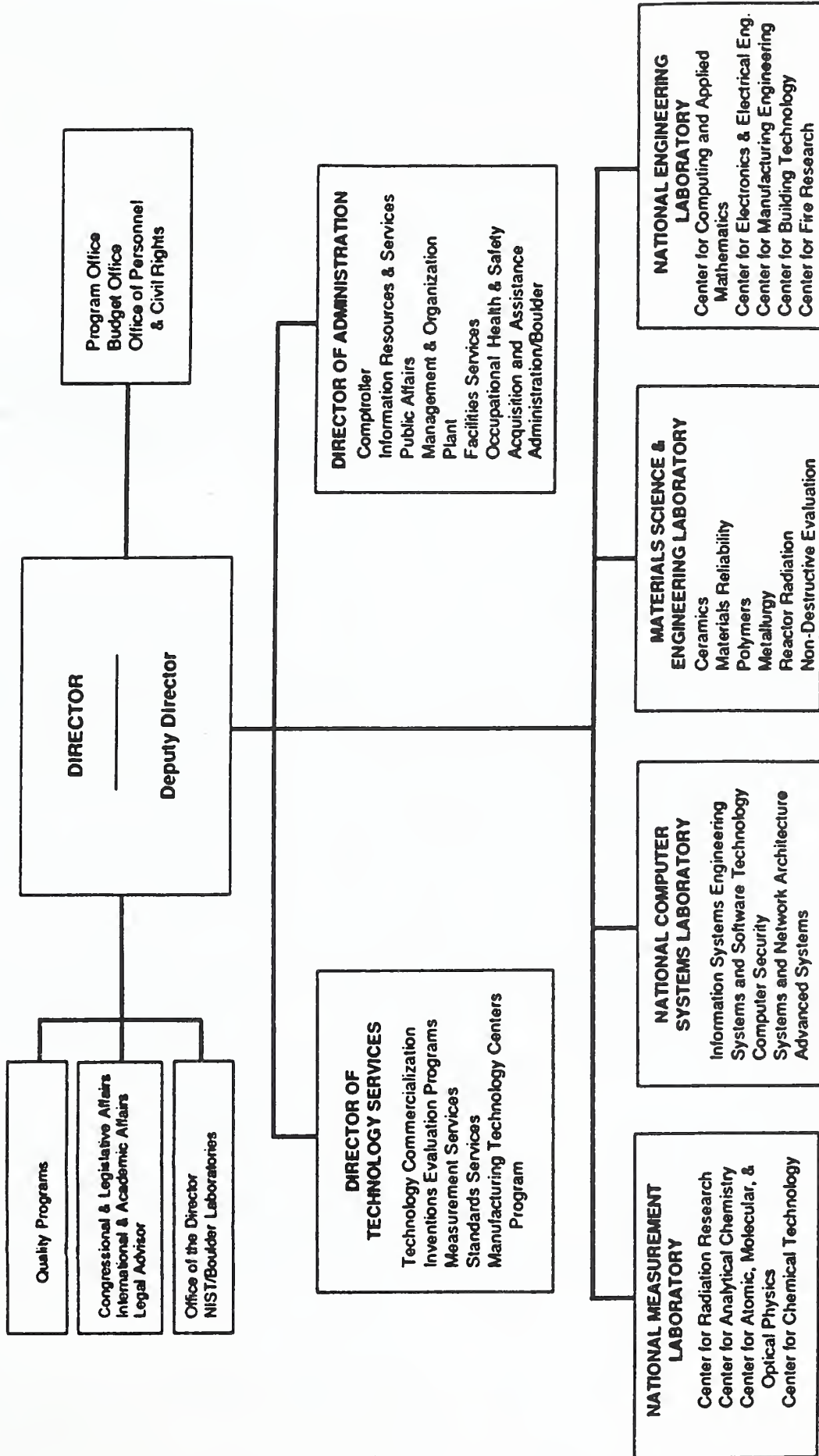
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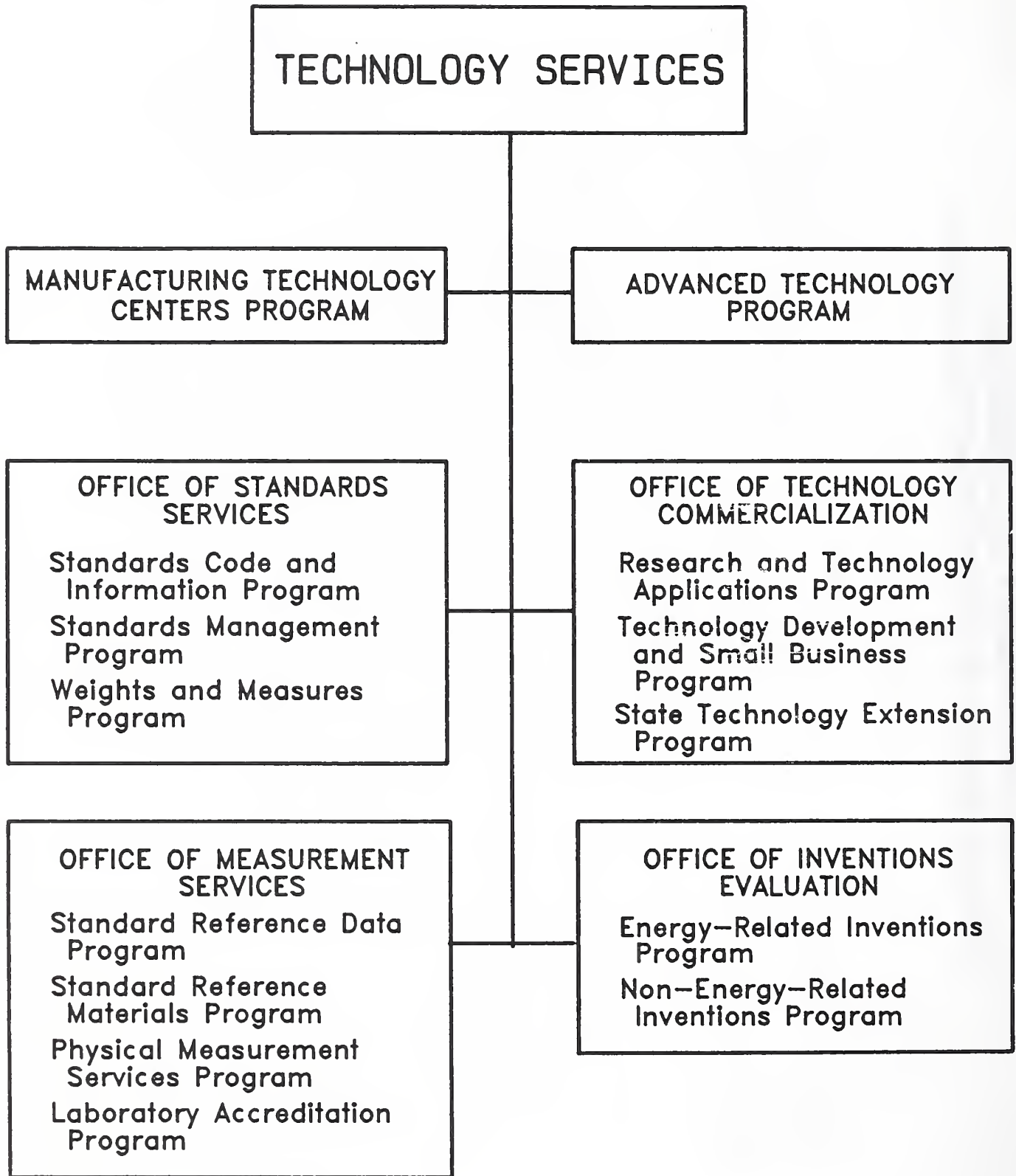
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* Standard Reference Data is not involved at the present time in the administration or funding of this data center but assists in making their outputs and services known to the scientific community. There is also considerable interaction between this data center and the Chemical Thermodynamics Data Center.

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11. ABSTRACT (A 200-WORD OR LESS FACTUAL SUMMARY OF MOST SIGNIFICANT INFORMATION. IF DOCUMENT INCLUDES A SIGNIFICANT BIBLIOGRAPHY OR LITERATURE SURVEY, MENTION IT HERE.)

Standard Reference Data is a program office in the Technology Services, National Institute of Standards and Technology. Standard Reference Data develops and disseminates publications and databases of critically evaluated physical, chemical, and materials properties of substances. These publications and databases are available through NIST and private publications, on magnetic tape, PC diskettes, and from on-line retrieval systems.

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 1989.

12. KEY WORDS (6 TO 12 ENTRIES; ALPHABETICAL ORDER; CAPITALIZE ONLY PROPER NAMES; AND SEPARATE KEY WORDS BY SEMICOLONS)

Chemical data; data compilation; evaluated data; materials properties data; numerical database; physical data; standard reference data; technical activities 1989.

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