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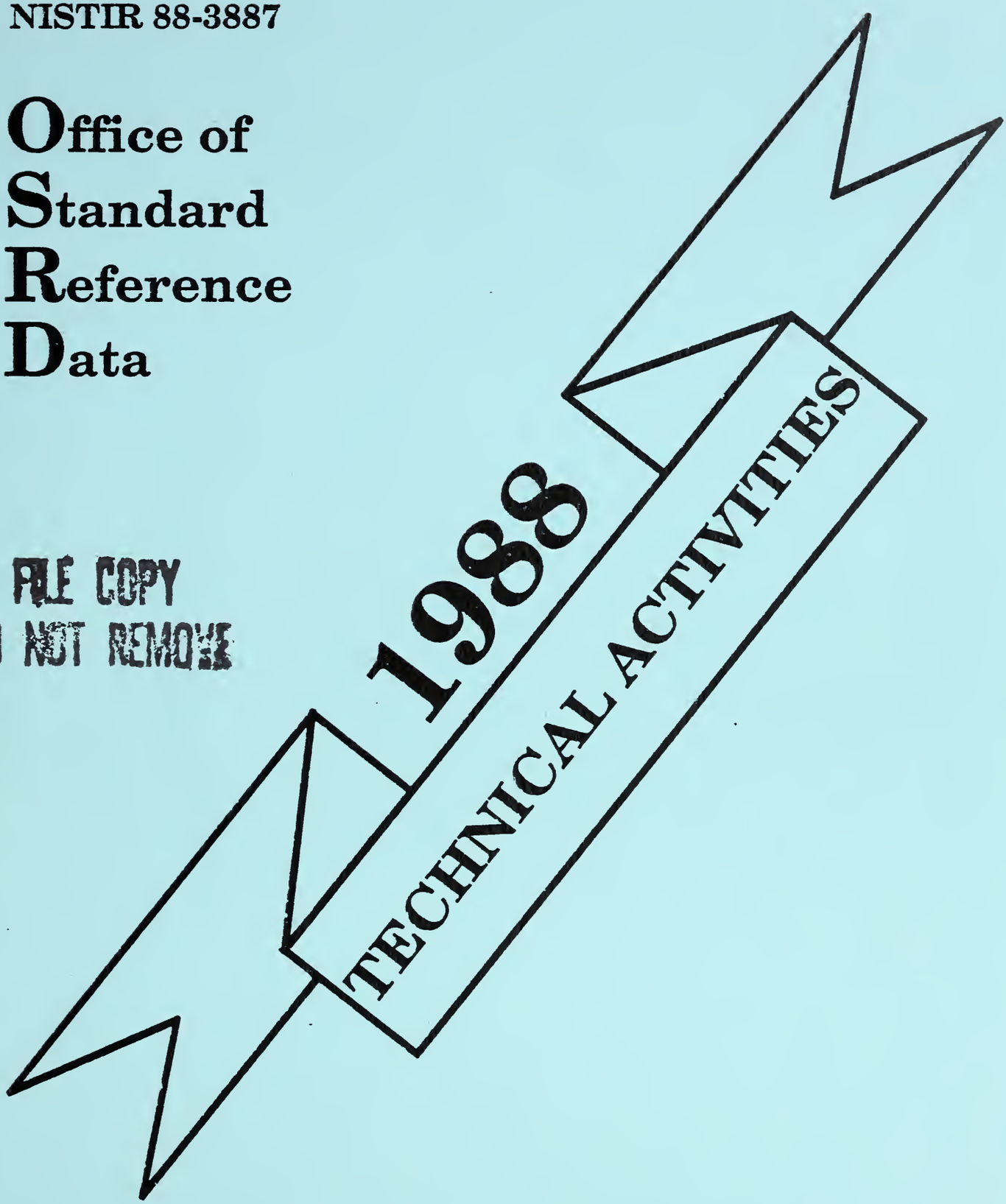
Office of Standard Reference Data



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Office of
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Data

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Technical Activities

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ABSTRACT

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

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1988.

Key words: Chemical data; data compilation; evaluated data; materials properties data; numerical database; physical data; standard reference data; technical activities 1988.

INTRODUCTION

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

The formal existence of the NSRDS dates from 1963, when the Federal Council for Science and Technology asked the National Bureau of Standards to assume primary responsibility in the Federal Government for promoting and coordinating the critical evaluation of numerical data in the physical sciences. The program was conceived as a decentralized national effort, with financial support coming from a variety of Government and private sources, but with NBS responsible for the overall planning and coordination. In 1968 the Congress provided a specific legislative mandate for the program through passage of Public Law 90-396, the Standard Reference Data Act. (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 materials of commerce (alloys, ceramics, etc.) whose composition may vary only within clearly stated ranges. Materials of uncertain or widely variable composition are not included. Properties which depend upon arbitrarily defined characteristics of the measurement technique are generally excluded. While these definitions leave many borderline cases, the overall intent is to concentrate the effort on intrinsic properties that are clearly defined in terms of accepted physical theory and substances whose composition and history are so well known as to justify evaluation of the data. Biological properties and data relating to large natural systems (e.g., the atmosphere, the oceans) also fall outside the program.

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

Journal of Physical and Chemical Reference Data - A quarterly 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.

NIST publication series distributed by the Superintendent of Documents, U.S. Government Printing Office.

Appropriate publications of technical societies and commercial publishers.

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

PROGRAM STRUCTURE

Current activities in the Standard Reference Data program are carried out in 21 data centers and approximately 40 short-term projects located in the technical divisions of NBS and in academic and industrial laboratories. Each of these activities undertakes the collection and evaluation of the available data on a specified set of properties and substances. The activities are aggregated into three discipline-oriented program areas:

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

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

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

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

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

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

Publications in 1988

Series	Pages Published	Titles Published
JPCRD, Vol. 17	3894	21
Data Compilations from other publishers	518	7
Other Publications in NBS Series	130	2
Bibliographies and indexes from other publishers	698	4
Total	5240	34

Subscribers to JPCRD

Month/Year	Number
9/1981	1265
9/1982	1234
9/1983	1230
9/1984	1186
9/1985	1160
8/1986	1087
9/1987	1076
9/1988	1047

Inquiries Received in OSRD

(Does not include inquiries received by data centers)

Year	Number
1981	657
1982	613
1983	1022
1984	616
1985	623
1986	926
1987	2172
1988*	2010

Sales of JPCRD Offprints and Supplements

Year	Offprints	Supplements
1981	4254	137
1982	3567	266
1983	3081	1666
1984	2900	1300
1985	3180	547
1986	2019	383
1987	1906	2222
1988*	3926	1376

*Projected to end of year

PHYSICAL DATA

S. G. Lias, Program Manager, October 1, 1987 - August 31, 1988
J. W. Gallagher, Program Manager, September, 1988

The Physical Data Program involves data centers and projects concerned with data from the discipline of physics, particularly the fundamental physical constants, atomic and molecular spectroscopy, and radiation physics. The program also includes the administration and development of spectral databases for use in analytical chemistry under a project called the Spectral Data Project.

The Physical Data Program

The data centers and currently active projects of the Physical Data Program and their areas of expertise are:

Fundamental Physical Constants

* Fundamental Constants Data Center (CAMOP): the fundamental physical constants and related precision measurements.

Atomic and Molecular Spectroscopy

* Atomic Energy Levels Data Center (CRR): energy levels and spectral lines of atoms and atomic ions.

* Atomic Transition Probabilities Data Center (CRR): radiative transition probabilities for atoms and atomic ions.

* Molecular Spectra Data Center (CCT): molecular spectral frequencies and other spectroscopic molecular constants.

* Project on Spectroscopic Properties of Excited Electronic States of Small Polyatomic Transient Molecules (CCT): a project for the compilation and evaluation of experimentally determined electronic energy levels of 470 neutral and ionic transient molecules, together with the associated vibrational structure, the radiative lifetime, the principal rotational constants, and literature references.

Radiation Physics

* Atomic Collision Cross Section Data Center (CAMOP/JILA): electron and photon collisional excitation and ionization of atoms and small molecules, heavy-particle energy transfer, photoionization, and photofragmentation.

* Photon and Charged Particle Data Center (CRR): the interaction of ionizing radiation with matter, including single-scattering

cross sections and transport data pertaining to the penetration of radiation through bulk matter.

The data compilations and evaluations provided by these data centers and the project are essential in such areas as laser physics, astronomy, astrophysics, plasma physics, fusion research, the utilization of electron beams in experimental physics, and in industrial and medical applications of radiation.

The details of the work of these data centers and projects, including goals, modes of operation, FY 88 accomplishments, and plans for FY 89 are given in the section entitled PHYSICAL DATA - DATA CENTERS AND PROJECTS.

Spectral Data for Analytical Chemistry

Under the same program, the Spectral Data Project is concerned with the administration and development of spectral databases for use in analytical chemistry. This project, unlike other "projects" funded by the Office of Standard Reference Data through one-time grants, is a long-range activity funded entirely by sales/leases of databases for analytical chemistry. In the past, the activity has not been associated with a traditional data center, but was jointly administered by the Program Manager in the Office of Standard Reference Data and outside collaborators. A major development during the past year has been the complete transfer to NIST of functions having to do with maintenance of the database, formerly carried out by the Environmental Protection Agency (EPA). A new Data Center is being established to handle the work of this project.

The NIST/EPA/MSDC Mass Spectral Database

The major activity under Spectral Data for Analytical Chemistry is the administration of the NIST/EPA/MSDC Mass Spectral Database. This collection of some 43,000 electron ionization mass spectra is put together from a larger archive of 80,000 spectra. The maintenance of the database is the joint responsibility of the National Institute of Standards and Technology (NIST), the Environmental Protection Agency (EPA) and the Mass Spectrometry Data Center (MSDC) of the Royal Society of Chemistry (England), which carries out the relevant literature search for locating new spectra.

In September 1987, the Office of Standard Reference Data released a searchable version of the database for use with personal computers. Because the new PC capability made the database more conveniently accessible to NIST scientists than it had been before, and because of the concerns about quality control of the database, a decision was made to bring the primary responsibility for the maintenance, evaluation, and updating of the database into NIST from EPA. During FY 1988, considerable effort was focused on developing the capability to do this. As a result, all of the functions necessary to producing a new edition of the Database can now be implemented on site at NIST. Although the EPA will continue to sponsor the Mass Spectral Database,

the role of that agency in the future will be to provide expert advice and original spectra from time to time.

The new data center, established on October 1, 1988, is called the NIST Mass Spectrometry Data Center, and is located in the Center for Chemical Technology. It will be jointly headed by Dr. Stephen E. Stein, who developed the PC version of the database, and Dr. Sharon G. Lias, who until September 1, 1988, was the OSRD Program Manager in charge of the project.

New Update of the NIST/EPA/MSDC Mass Spectral Database: A new edition of the database, to be released both on tape and in a PC version, is being prepared at this writing. For the first time, the database will include structural information on approximately 90 percent of the compounds for which spectra are given. New spectra available for the 1988 update are: 5,286 spectra from the Mass Spectrometry Data Center, 2,750 spectra from an international exchange with the Soviet Union, 400 spectra donated by individuals, and 4,200 spectra from the archive for which Chemical Abstracts Registry Numbers have been obtained. The spectra are added to the database with new quality control procedures and error checks applied to the data as they are added. Work on retrieving Registry Numbers is continuing at this writing. The availability of these 13,000 spectra does not necessarily mean that the size of the database will increase by this amount, since undoubtedly some of the relevant compounds are already represented in the database, and replicate spectra of a given species are not included.

The PC Version of the NBS/EPA/MSDC Mass Spectral Database: On September 21, 1987, a fully searchable PC version of the database with seven search options was released for sale to the public at a price of $750 per copy. This version includes a listing of the complete spectrum, a "10-peak index" giving the largest 10 peaks in order of abundance, a graphic display of the spectrum, plus lists of numerous synonyms for the name of the compound (all fully searchable). By the first of September 1988, 65 copies had been sold through OSRD. In addition, the Mass Spectrometry Data Center signed an agreement as a distributor of the PC version in Europe, and they had reported the sale of several copies at the 11th International Mass Spectrometry Meeting in Bordeaux, France, during the first week of September.

A review appeared in the Journal of the American Chemical Society (J. Am. Chem. Soc. 110, 3336 (1988)) which praised the speed and flexibility of this PC database. It is anticipated that as mass spectrometrists become increasingly aware of its existence, the rate at which copies are sold will increase greatly.

After the initial release in 1987, work was begun on the development of more sophisticated search software which would fully utilize the capacities of modern personal computers. Connection

tables were obtained which provided structural information about 85 percent of the compounds in the database, and software was written to permit the display of structural drawings. Structural information for most of the remaining 15 percent of the compounds was entered into the database. A new release which incorporates the new update of the database along with the structural information and several new search options is planned for November 1988.

The Magnetic Tape Version of the NBS/EPA/MSDC Mass Spectral Database: The database is distributed both on tape and in the PC version. The tape version is mainly leased by manufacturers of mass spectrometric instruments for use in the data systems of instruments. With release of the new update, the tape version will also include the structural information about the compounds in the database.

Improvements in Quality Control of Spectra in the Database: The database of approximately 43,000 spectra is put together from a larger archive of 80,000 spectra. This archive includes every spectrum ever acquired for the database since its beginning in 1968 at EPA. Over the years, a number of mistakes (misidentified spectra, incorrect formulas, etc.) have crept into the archive, and occasionally some of these have made their way into the database which is distributed to the public. In November 1987, the archive was transferred to NIST from the EPA computer in Triangle Park, North Carolina. Programs were completed by December to transfer the information to the hard disk of a personal computer. Special programs for searching and editing the archive were written and work was begun on locating and editing or deleting bad spectra. For the fall 1988 update, attention was concentrated on eliminating all obvious errors in the spectra eligible for inclusion in the distributable version (i.e. spectra associated with a Chemical Abstracts Registry Number). A continuing effort will involve surveying the entire archive with the goal of eventually eliminating or flagging all incorrect or marginally correct spectra, and obtaining Registry Numbers for several thousand spectra in the archive. The Quality Index calculation has been adapted for use on the personal computer; future editions of the database will display not just a single grade for each spectrum, but a breakdown of the various items on which a spectrum is graded (instrument conditions, presence of peaks due to impurities, etc.), so that a user can understand the origin of the Quality Index value.

Publication of New Hard-Copy Version of the Database: The set of volumes with copies of the spectra appearing in the 1987 edition of the Wiley/NBS Registry of Mass Spectra is in press, and will appear in the late fall of 1988.

Expansion of the Spectral Database Project

Infrared Spectra: The NBS/EPA Interagency Agreement of 1985, put in place to govern the joint administration of the NBS/EPA/MSDC Mass Spectral Database, specified that the two agencies would investigate the need for and feasibility of development of a database of infrared spectra. In October 1986, the EPA made a grant to Drs. Peter R. Griffiths and Charles L. Wilkins, both of the University of California at Riverside, to (1) develop a computerized algorithm for the evaluation of infrared spectra, and (2) collect digitized reference spectra from contributors with the purpose of creating an evaluated database of IR spectra. Drs. Griffiths and Wilkins have expressed interest in having OSRD eventually serve as the distributor of the database.

M. W. Chase, Program Manager

The chemical data program of the Office of Standard Reference Data refers primarily to data describing the physical properties of individual substances and mixtures and data describing chemical reactions between substances. Both categories cover equilibrium and time-dependent properties; thermodynamic and transport property data (such as viscosity and thermal conductivity) in the case of the individual substances and mixtures, and thermodynamic and rate data in the case of the chemical reactions.

The descriptive data on substances used in analysis and identification and in selection of materials based on their predicted behavior is not covered in this section. To some extent, these are covered in the section on physical properties, 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 involves the thermodynamic data for the substances involved, although it is covered largely under material properties. 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 work on chemical data is carried out in data centers and data projects. Data centers are continuing in nature. Their staffs take responsibility for continuing coverage of the data in their fields of specialization and produce a continuing 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 principal areas of coverage 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 the Office of 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 OSRD, 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

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

Table 2

Data Projects in the NSRDS Program for Chemical Data

Thermophysical Data

Thermophysical Properties Data for Fluids, University of Maryland
Equations of State for Mixtures of Argon, Nitrogen, Oxygen and of Air, University of Idaho
Equilibrium and Transport Properties of Polyatomic Gases and their Mixtures, Brown University
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
Thermochemistry, Inc., Oklahoma State University
Application of Expert Systems to Critical Evaluation of Thermophysical Property Data, Texas A&M Research Foundation

Chemical Thermodynamic Data

Data on Aqueous Electrolytes, University of Delaware
Gibbs Energies of Formation for Kreb's Cycle and Related Compounds, University of California, San Diego
Design Institute for Physical Properties Data, AIChE

A Centralized Database for Thermodynamic Data on Lipid Mesomorphic Phase Transitions and Miscibility, Ohio State University

Chemical Kinetics

Properties of Transition Metal Coordination Complexes, Boston University
OH Radical Reactions with Organic Compounds, University of California, Riverside

The program in thermophysical properties is concerned primarily with fluids. Both thermodynamic and transport properties are included.

Chemical thermodynamic data include the Gibbs energies and enthalpies of formation of substances from the elements in their standard state as well as the entropies of the substances and their heat capacities, all at standard conditions. In addition, thermal functions are given so that it is possible to determine the formation properties of substances, and hence the equilibrium constants and enthalpies of reactions involving them over the range of temperatures covered. The substances covered are inorganic and organic molecules. Special attention is given to aqueous electrolyte solutions. Activities over the available range of concentration are provided.

Chemical kinetics data include data for homogeneous gas-phase reactions, gas-phase reactions involving ions and radiation chemistry, and photochemistry in solution.

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. 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. OSRD and DIPPR

cooperate in a number of ways. OSRD sponsors DIPPR, carries out selected projects for DIPPR and acts as distributor for automated products for DIPPR. OSRD 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 data centers 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. One book of results from this task group has been published, another is in press 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, is expected to be published in early 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 by OSRD, 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 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. Tables may be submitted in camera-ready 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

The output of the program will be listed in detail at other places in this report. As a brief summary, 7 books were published in the past year which in one way or another contained output resulting from the activities of the program. Not all of these are considered OSRD products but all result from sponsored or cooperative activities. There have also been 3 automated databases produced and 9 papers and two supplements in JPCRD as well as papers in other journals and reports.

MATERIALS PROPERTIES DATA

John Rumble, Jr., Program Manager

Several major milestones were accomplished in 1988 in the Materials Data Program.

* Update of the NIST Crystal Data File

* Completion of phase 3 of a materials data network (with the MPD Network)

* Completion of the first expert system for a NIST data project (with NACE and MTI)

* Organization of the First International Workshop on Standards for Materials Databanks (with VAMAS)

* Release of a fatigue data evaluation package for PC's

* Publication of new monographs on Alloy Phase Diagrams

* Publication of first SRD article on evaluation of fracture toughness data

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 six 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

Society	Data Area
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 1988, great progress has been made.

Let us touch upon the highlights within each component; new areas of activity will be pointed out.

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 1988, now has data on over 115,000 compounds. The database comes with software to analyze experimental measurements and then search the database for matching entries. Negotiations are going on 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 - 1988

Structure and Characterization
- Crystallography
  - NIST Crystal Data Center
  - Cambridge Crystallographic Data Centre
- Surfaces
  - ESCA Data Project - Surfax (CA)
  - Ion Sputtering - NBS
  - 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
- Ductile Fracture Toughness of Low-Alloy Steels - University of Florida
- Fracture Toughness of Aluminum Alloy - MPD Network

Tribology
- Tribology Information Activity - NIST

The characterization of surfaces is the other major component of this part of the program. The SRD compilation for low-energy electron diffraction (LEED) is being incorporated into a database. LEED is a widely used technique, and this database will be widely used too.

Projects on ESCA and ion-sputtering data are in the last stages of completion. A prototype ESCA database was prepared this year and is being readied for distribution. 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, but a subpanel of the Numerical Data Advisory Board has been looking at data needs related to high-tech materials. Their recommendations will be issued soon and should recommend new emphasis on optical and electronic properties.

A project on polymer-polymer miscibility at RPI under the direction of Professor Krause is moving ahead.

A project on properties of glassy-forming melts has moved into 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. SRD is studying how best to continue cooperation in this area.

Phase Equilibria

NIST, through the Institute for Materials Science and Engineering (IMSE) 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 7 of its series Phase Diagrams for Ceramists as part of the joint program with the American Ceramic Society. About 700 critical evaluations and over 1000 individual phase diagrams are included.

A PC database and graphics program for ceramics phase diagrams has been completed and is now undergoing testing by ceramists. The database will be sold beginning in 1989.

The ASM/NIST Alloy Phase Diagram Program has continued, and over 1300 binary alloy systems have been evaluated and more than 700 published.

During 1988, NIST changed the way technical editing for the Bulletin of Alloy Phase Diagrams is provided, and Professor Jack Smith of Iowa State is now under contract to act as editor.

Performance Properties

Corrosion

The NACE-NIST Corrosion Data Program has two databases, both based on the NACE Corrosion Data Surveys. One database covers metals, the other nonmetallics. Both are PC-based and represent comprehensive collections of corrosion rate data.

The Data Center is moving ahead with other database projects involving collection of corrosion data sets from industry and their evaluation for reliability and quality. The first set to be transferred is from the LaQue Center for Corrosion Technology, and the Data Center is presently analyzing the data. A prototype database has been prepared and will be sent to outside reviewers in late 1988 for testing. Final release will be in early 1989.

In addition, the NACE-NIST program has begun developing 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. This will be distributed to MTI's members in 1989 for their use.

Mechanical Properties

The SRD effort on mechanical property 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.

A compilation of fracture toughness data done by Professor Ebrahimi of the University of Florida was published in the ASTM Journal of Testing and Evaluation early in 1988.

In 1988, distribution was made of data evaluation software built by Susan Foss of John Deere Company under grants from SRD. This software has been distributed to over 50 groups doing fatigue data analysis. A publication on the methodology is scheduled for early 1989.

Tribology

A multi-agency program for tribology data, started in 1986, is now well underway. NBS 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, and SRD is represented on the Board of Directors.

During 1988, SRD programmers have put together the first product of this effort, a database package that contains four well-evaluated data sets. The database has been completed and demonstrated, and distribution arrangements are being made.

Computer Access and Databases

The strong SRD effort to help bring about computerization of materials data has continued, and major accomplishments were achieved in 1988. Several database efforts have already been discussed. Other areas deserve mention.

SRD and the MPD Network have worked together to complete Phase 3 of a materials data network. Two demonstrations were held in September 1988, and the new system is now available to selected users in industry and federal labs.

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 and the VAMAS Technical Working Group 10 on Factual Materials Databanks.

During 1988, ASTM Committee E-49 has developed and balloted 15 separate standards, and more are being written. Also, SRD has worked with VAMAS to hold an international workshop in November 1988 to implement recommendations made in an earlier VAMAS report. That comprehensive survey of standards needs is providing guidance to standards development throughout the world.

Summary

Despite minimal resources, the SRD program on Materials Properties Data remains strong and is moving in new directions. The year 1989 promises even more accomplishments.

COMPUTERIZATION

B. B. Molino, Group Leader

The major commitment by the Office of Standard Reference Data to automate the internal operations of its data centers and to develop numerical databases for dissemination in various formats has continued throughout the past year.

The level of activity in these areas was able to be increased when we were awarded funding ($500K) for the FY88 initiative, Computerized Reference Data. Progress made in the various areas of effort are summarized below.

Computing Facilities

We continue to provide stable, state-of-the-art hardware, software, communications, and support to our data centers and data projects, as well as for the central functions carried out in our own office. A substantive upgrade to the SRD Computer Facility was procured as a major part of the budget initiative on Computerized Reference Data, as mentioned above. This upgrade is in keeping with the long-range plan outlined previously to this panel, and provides our users with a very much more powerful machine, the Hewlett Packard 840. This machine has the important capabilities of a 32 bit word, additional memory (16 MB), faster processing, and an industry standard UNIX operating system. This operating system is extremely important to our efforts since it allows us the use of built-in utilities, it provides a wider selection of third party software, it permits communication with much of the outside world, and it is compatible with the operating system of our existing composition system.

By upgrading to a machine from Hewlett Packard, we were able to retain and to interface to existing peripherals, including terminals, printers, and tape drives. This also ensured the transportability of our substantial investment in software for database automation and in database dissemination procedures with minimal effort. Indeed, due to the careful planning and painstaking benchmarks done by the Data Systems Development staff, the transition to the new facility went smoothly and with very minimal (about 2 days) downtime.

Two related procurements to this upgrade are significant enough to deserve individual mention. The first is the purchase and installation of the database management package ORACLE. This distributed DBMS runs on mainframes, minis, and micros. It is a product of the fastest growing software company, and has advantages such as allowing applications larger than the typical 640K and providing for a more sophisticated multiuser environment. We have several applications up and running in ORACLE, and will be happy to demonstrate them. Multiple other projects are underway using this product.

The second significant procurement is that of a high performance plotter and associated software. This HP 7596a plotter with the associated

GRAFIT software package is expected to enhance the data evaluation activities required to prepare databases to support emerging technologies. In addition, it will increase our options for data presentation in computerized formats, and will enhance our present publication procedures.

As part of the enhancement of the SRD Computing Facilities, we have maintained currency with the state-of-the-art microcomputer capabilities. Each SRD staff member has a personal computer for his or her use, and we have both added to the number of microcomputers in the office and enhanced existing machines with additional memory, storage, and peripherals, including a Bernoulli box. We now have multiple IBM PS/IIs - two with 60 megabytes of storage and the 20286 chip and one (as recommended by the Evaluation Panel last year) with 80 megabytes of memory and the 20386 chip.

The list of newly acquired software for these personal computers is also impressive and includes:

Professional ORACLE
Professional ORACLE support
REVELATION
RGRAPH
dBASE III upgrade
WORDPERFECT
WORDSTAR
SMARTCOM II
REFLECTIONS terminal emulation
CLIPPER upgrade
Ryan McFarland FORTRAN upgrade
MICROSOFT C upgrade

We keep abreast of developments with the NBS Consolidated Scientific Computing System $(CS)^2$, and through representation on the User Committee for Scientific Computing we provide input as to what we feel are desirable hardware and software features for the SRD program with which to enhance the present machine or which to include in future procurements.

With these increased computer facilities, and through the diligent efforts of the Data Systems Development Group, we continue to work towards propagating common automation techniques across data centers, to promote standardization and integration whenever possible, and to reduce any duplication of effort. Along these lines, we held a very successful data center workshop on chemical databases to discuss common techniques, problems, and concerns, we offered an indepth C programming course for SRD and data center staff, and the Data Systems staff provides mini-courses on machine-specific features as well as individual consulting.

Publication Procedures

The Bedford Composition System for computer typesetting of our publications is operating smoothly. We continue to realize a reduction in the amount of processing required in this office as well as a reduced turnaround time, and even publications from data centers outside NIST are

processed with relative ease. Because of the efficiency and high quality of this system, we were able to typeset 2000 pages and 1200 page templates. This includes the impressive list of 3 JPCRD supplements, 9 JPCRD articles, 1 book, and miscellaneous documents.

Improvements to the operation of the NIST Bedford Composition System during the past year are as follows:

Hardware:

PC for communications
tape streamer for back-up
surplus equipment and spare parts from GPO

Software (purchased):

operating system updates
script font capability

Software (developed in-house):

conversion routines from word processors to Bedford
conversion routines from Bedford to ASCII
template design for page make-up

The processing of many publications is streamlined by using the enhanced laserjet printers associated with the SRD Computing Facilities. In addition, programs are being developed to facilitate the processing of tables for output to the laser printer, and to reformat data with appropriate mark-up for typesetting through the Bedford System.

Numerical Database Activity

In the area of numerical database dissemination, we are proud to announce the release of DDMIX (Database 14), an interactive program package to calculate various thermodynamic and transport properties of mixtures or pure fluids selected from any of 17 possible pure components. In addition, the DIPPR Data Compilation of Pure Compound Properties (Database 11) has now been updated to include 766 chemical compounds, more than double the number in the previous version containing 346, and a diskette version of this database is now available.

Numerous PC databases are in the final stages of development, and will be released in the near future. Many of these are being funded from the 1988 Computerized Reference Data initiative funds, and include:

Electronic and vibrational energy levels of transient molecules
Electron stopping power database
Photon attenuation database
Chemical kinetics database
Ion energetics database
Prediction program for thermochemical properties of hydrocarbons
Thermophysical properties of fluids for use as refrigerants
NBS chemical thermodynamics tables

The number of inquiries and orders for all our databases continues to rise steadily.

A complete listing of the present NIST Standard Reference Database Series along with the number of each sold in 1988 follows:

NIST STANDARD REFERENCE DATABASE	1988 Sales as of November 3
1. NBS/EPA/MSDC Mass Spectral Database	2
1A. NBS/EPA/MSDC Mass Spectral Database: PC Version	67
2. NBS Chemical Thermodynamics Database (NBS Tech Note 270)	3
3. NBS Crystal Data Identification File[1]	
4. NBS Thermophysical Properties of Hydrocarbon Mixtures (TRAPP)	0
7. Electron and Positron Stopping Powers of Materials	3
8. X-ray and Gamma-ray Attenuation Coefficients and Cross Sections	6
9. Activity and Osmotic Coefficients of Aqueous Electrolyte Solutions	1
10. Thermophysical Properties of Water (STEAM)[2]	2 (tape) 5 (diskette)
11. DIPPR Data Compilation of Pure Compound Properties[2,3]	9 (tape) 4 (diskette)
12. Interactive FORTRAN Programs to Calculate Thermophysical Properties[2] of Fluids MIPROPS	1 (tape) 19 (diskette)
13. JANAF Thermochemical Tables	9
14. Mixture Property Program-DDMIX[2,3]	24 (diskette)
15. NBS/Sandia/ICDD Electron Diffraction[1]	
16. Corrosion Performance Database[4]	

[1]Available from the JCPDS-International Centre for Diffraction Data, 1661 Park Lane, Swarthmore, PA 19081. Phone: (215) 328-9400.
[2]Also available in diskette form (same prices apply).
[3]Discount available to members of DIPPR. Discount available to GPA Members for DDMIX.
[4]Available from NACE, P.O. Box 218340, Houston, TX 77218 Phone: (713) 492-0535.

Also, we continue to press for the inclusion of our numeric files in on-line systems. We have been working very closely with the technical staff at Chemical Abstracts Service and are pleased to announce that two of our databases, the JANAF Thermochemical Tables and the NBS Chemical Thermodynamics Database, are now available on STN. Presently, the Mass Spectral Database, the Chemical Thermodynamics Database, and the Crystal Data Identification File are resident on CIS, Mass Spec is also available on Questel and JICST, and the CISTI System offers the Crystal Data Identification File.

We were pleased to be able to demonstrate many of our databases at various national and international meetings. At the Third North American Chemical Conference in Toronto, Canada, in June, we organized a demonstration session entitled Computerized Dissemination of Numerical Data for Chemists which featured many of our databases. In addition, Data Systems staff members demonstrated our databases at the Pittsburgh Conference and Exposition on Analytical Chemistry and Applied Spectroscopy in New Orleans, in February, the Thermophysics Symposium held here in June, and at the World Materials Congress in Chicago, in September.

Database Activities

Individual data centers continue to make great progress in their database efforts and to work closely with DSDG to ensure standardization and compatibility whenever possible.

Our commitment to the automation of the numeric data files for the Atomic Energy Levels Data Center and the Atomic Transition Probabilities Data Center continues. With the availability of the new computer resources, we did a detailed analysis, and determined that this automation project could best be accomplished using the ORACLE database management system. During the past year, we completed the database design, converted existing data files into a format to be loaded, and proceeded to load a large sample of records. We now have a prototype ORACLE database containing approximately 5000 energy levels, and have developed interfaces to make standard reports and to process energy data for printing. Presently we are designing and implementing data entry screens and updating programs.

Conversion of existing automation activities to the new machine is complete. New projects from additional data centers are now in progress, making use of the availability of the enhanced hardware, software, and communications of the new computer facilities.

Reference Center Automation

We maintain current files of Reference Center holdings and JPCRD articles, including property and material terms, on the OSRD computer facility. This, in coordination with appropriate interfaces to the Bedford Composition system for computer typesetting, continues to facilitate the preparation of publication lists and other documents. Other automated activities associated with the Reference Center include a tracking system for the review and production processes of publications in progress, a computerized coded mailing list, and a dBASE III database of tape sales.

Outside Interactions

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

DATA CENTERS

ATOMIC COLLISION CROSS SECTION DATA CENTER

Director: Jean W. Gallagher
Center for Basic Standards, NIST

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

In the past year, two evaluated data compilations were completed and are ready to be submitted for publication. These include: (1) "Review of Experimental Optical Excitation Functions," by D. W. O. Heddle and Jean W. Gallagher; (2) "Collision Cross Sections for Ions and Neutrals in Parent Gases: Ar, N_2, H_2" by A. V. Phelps. In addition, the article "Absolute Cross Sections for Molecular Partial Photoionization and Photofragmentation Processes" by J. W. Gallagher, C. E. Brion, J. A. R. Samson, and P. W. Langhoff was published in the Journal of Physical and Chemical Reference Data. The article, "Collisional Alignment and Orientation in Atomic Outer Shells. I. Direct Excitation by Electron and Atom Impact," by Nils Andersen, Jean W. Gallagher, and Ingolf V. Hertel was accepted for publication in Physics Reports. Work continues on parts "II. Quasimolecular Excitation" and "III. Spin-resolved Excitation" of this series.

Work continues on development of and entry of data into the Atomic Collision Cross Section Data Base (ACDB). Over 20,000 records have been collected in Index-Sequential files over the last 10 years. Approximately 70 percent of these data are suitable for the ACDB. Work has begun on reviewing the data and transmitting them to the ACDB, and approximately 500 data records have been added.

New data entry software for use with personal computers has been completed. Use of this software will increase the efficiency of data entry and ensure that identifying material in files destined for the Data Base is complete and accurate. Work continues on the interactive retrieval program for the Atomic Collision Data Base.

In addition to the continuing projects listed above, plans for the coming year include (1) the identification and collection of papers on cross sections for electron collisions with small molecules; (2) an update to "An Evaluated Compilation of Data for Electron Impact Excitation of Atomic Ions" by J. W. Gallagher and A. K. Pradhan, published in 1985, is planned.

ATOMIC ENERGY LEVELS DATA CENTER

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

The critical compilation and evaluation of energy levels for all 42 spectra of molybdenum, "Energy Levels of Molybdenum Mo I through Mo XLII" by J. Sugar and A. Musgrove, was published in the Journal of Physical and Chemical Reference Data. Significant progress has been made on a similar compilation for the 29 spectra of copper. In addition, a critical review and compilation of data for all scandium spectra, Sc I through Sc XXI, has been completed. A collaboration with Japanese physicists has produced compilations of wavelengths, energy-level classifications, and Grotrian diagrams for 19 iron spectra (Fe VIII-XXVI). A similar compilation for 19 spectra of chromium (Cr VI-XXIV), which are of special interest for fusion research, is nearing completion.

A fourth supplement to the Bibliography on Atomic Spectra covering the literature from January 1984 through December 1987 is in press for publication later this year.

In addition to the activities mentioned above, future activities include the compilation of wavelengths and energy-level classifications for the silicon spectra, Si I-XIV, energy-levels of sulfur spectra, and the initiation of a critical compilation of calcium spectra.

ATOMIC TRANSITION PROBABILITIES DATA CENTER

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

The preparation for publication of the data on atomic transition probabilities for the iron group elements scandium through nickel in all stages of ionization is nearing completion. The two-volume compilation will appear in late fall, 1988.

An annotated bibliography on "Atomic Transition Probability Data for Astrophysics and Space Physics," which covers the literature for the past three years will be published in the 1988 "Reports on Astronomy".

Future plans call for beginning the compilation of critically evaluated transition probability data on the elements hydrogen through neon. This will be a complete revision of an earlier compilation, published as NSRDS-NBS 4, which first appeared in 1966 and is now hopelessly out of date. Because there have been numerous major theoretical and experimental developments since that publication appeared, this will be a major undertaking which will occupy the primary attention of the Data Center for several years. New theoretical data resulting from the so-called "Opacity Project" have been tested against very accurate experimental data for singly ionized and doubly ionized carbon, and have been found to be in excellent agreement; the new compilation will include the new theoretical data.

FUNDAMENTAL CONSTANTS DATA CENTER

Director: Barry N. Taylor
Center for Basic Standards, NIST

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

The principal focus of the Center during the past year has been (1) the continued wide dissemination of the 1986 adjustment and recommended values of the fundamental physical constants, and (2) work on the 1988 Conference on Precision Electromagnetic Measurements (CPEM) at which new results relating to the fundamental constants were presented and subsequently used to develop improved best values for the Josephson frequency-voltage ratio $E_J = 2e/h$ and quantized Hall resistance $R_H = h/e^2$. The Center actively participated in meetings of the CODATA Task Group on Fundamental Constants as well as the E_J and R_H Working Groups of the Consultative Committee on Electricity, CIPM.

A detailed paper for the Journal of Physical and Chemical Reference Data on data analysis pertaining to the 1986 adjustment of the fundamental constants is being prepared.

MOLECULAR SPECTRA DATA CENTER

Director: Frank J. Lovas
Center for Chemical 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 of a wide range of molecular properties. One phase of the Center's work emphasizes microwave spectra of interstellar molecules.

Part III of the Microwave Spectral Tables was submitted for publication in the Journal of Physical and Chemical Reference Data. This critical review, which includes 130 tables of molecular constants and 95 tables of spectral frequencies, contains all of the rotational spectral lines observed and reported in the literature for 91 hydrocarbon molecules.

Work has begun on Part IV of the Microwave Spectral Tables, which will treat organic species containing oxygen. Our reprint files contain about 157 species in this group with empirical formulas CHO to $C_7H_{12}O$. Spectral data for the first 25 species have been coded for spectral fitting and table generation.

The update of the publication "Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions - 1985 Revision" is planned for 1989. Since the last revision was published, 15 new interstellar species have been identified, bringing the number of identified molecules to 74.

PHOTON AND CHARGED PARTICLE DATA CENTER

Director: M. J. Berger
Center for Radiation Research, 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 database and program called XGAM, which is usable on a personal computer, was submitted for internal review prior to release for distribution. This program provides X-ray attenuation coefficients and individual cross sections for photon scattering, absorption, and pair production at energies from 1 keV to 100 GeV for any element, compound, or mixture. This program is the successor to an earlier mainframe program XGAM, and is different not only in format but also in the use of updated cross sections.

A database and program called EPSTAR has been developed. This program can be used to calculate on a personal computer, electron and positron

stopping powers and ranges, density-effect corrections, and bremsstrahlung yields at energies from 10 keV to 10 GeV for any element, compound, or mixture.

Systematic calculations have been completed of the cross section for the elastic scattering of electrons by atoms at energies from 1 keV to 1 MeV for all elements, Z = 1 to 100. The entire body of data has been processed into an organized database which can be queried on a personal computer. In addition, the cross sections for electron bremsstrahlung production for all elements, Z = 1 to 100 at energies from 1 keV to 10 GeV, have been organized as two computer files. A program for accessing this information on a personal computer is being completed. These databases are important for the utilization of electron beams in experimental physics and in industrial and medical applications.

A paper entitled "National Bureau of Standards Data Base of Photon Absorption Cross Sections from 10 eV to 100 GeV" was presented at SPIE Conference 911 (Los Angeles, January 1988), and will appear in the proceedings of that conference.

Plans for the coming year include (1) updating the 1972 comprehensive evaluation of energy absorption coefficients, data which are important for industrial and medical dosimetry; (2) generating comprehensive and up-to-date tables of alpha particle stopping powers and ranges for compounds of interest in radiation protection dosimetry, for use in evaluating the effects of radon in houses; (3) extending the calculations for the elastic scattering of electrons by atoms to energies above 1 MeV using screened Coulomb potential-derived relativistic Hartree-Fock wave functions.

PROJECTS

SPECTROSCOPIC PROPERTIES OF EXCITED ELECTRONIC STATES OF SMALL POLYATOMIC TRANSIENT MOLECULES

Marilyn E. Jacox
Center for Chemical Physics, NIST

A major data compilation, entitled "Electronic Energy Levels of Small Polyatomic Transient Molecules," was published (M. E. Jacox, J. Phys. Chem. Ref. Data 17, 269-511 (1988)). This compilation and an earlier one, entitled "Ground-State Vibrational Energy Levels of Polyatomic Transient Molecules" (M. E. Jacox, J. Phys. Chem. Ref. Data 13, 945-1068 (1984)) are being supported by the continuing evaluation and addition of more recent experimental data. It is planned to prepare a supplement for publication during FY '89.

A project concerned with the preparation of computer-accessible files based on the data in these compilations received support from OSRD. The first part of this project, the preparation of an ASCII version of these tables suitable for on-line data access, has been completed. With the help

of a summer worker, substantial progress has been made toward the achievement of a second goal of this project, the preparation of compiled dBase III+ files of the values of the electronic band origins and vibrational fundamentals in these tables. These two files will permit searches over user-specified wavenumber or wavelength ranges. Searches can be further restricted to molecules containing certain elements. A dBase III+ file of all of the vibrational fundamentals for small polyatomic transient molecules with from 3 to 6 atoms in their ground and excited electronic states is complete and contains 4378 entries. Data for the electronic band origins have been reduced to a tabular form which can readily be converted to dBase III+ after minor editing has been performed. Material to be published in the supplement is being included in the ASCII and dBase III+ files concurrently with its addition to the compilation.

The compilation is now being prepared for distribution as a personal-computer accessible database.

DATA CENTERS

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 for 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. Frequently cited examples of the need for electrolyte data are the design of efficient chemical plants, the study of environmental fates of industrial wastes, and the modeling of corrosion processes in power cycles.

A new area of interest is the evaluation of existing data on and the modeling of the properties of solutions containing ionic surfactant and highly polar solutes such as alcohols and amines which are used in many industries.

Among the significant accomplishments during the past year are: developed the computer code required to fit experimental measurements over wide ranges of T, p, and x; designed and implemented a computer readable bibliography on the thermodynamic properties of the KCl-H2O; completed a personal computer version of the Aqueous Thermodynamics Data Base (initial documentation of the versions of this program for personal- and minicomputers were circulated within NIST earlier this year); reviewed the GAMMIX program (as developed by Professor Robert Wood and William Davis) for the calculation of activity and osmotic coefficients; designed and implemented a PC-version of the NBS Tables of Chemical Thermodynamic Properties.

As part of a contract with the Design Institute for Physical Property Data, DIPPR, a program called GAMMA was written to permit the retrieval of activities and osmotic coefficients for a moderate range of temperatures above room temperature. GAMMA runs on the CTDC HP-1000 minicomputer and currently is being converted to run on personal computers.

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 sub-sets 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.

The evaluated chemical kinetic database for combustion chemistry has been expanded during the past year. The original data for methane has been extended to include methanol, C3 alkanes and alkyl radicals, and C4 alkanes and alkyl radicals. Also data for the reactions of isobutyl and propene are being evaluated.

Other activities include the following. The compilation of chemical kinetic data for combustion chemistry is a much larger database than the comparable evaluated database, containing upwards of 1900 elementary reactions. This is the core database that will be used for the development of a general database containing data on all gas phase chemical reactions. The center continues to provide 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). The analysis of dielectric breakdown and chemical vapor deposition (plasma chemistry) have received continued attention, with a consideration of the thermal stability of sulfur hexafluoride and disulfur decafluoride. All data activities involving the use of the HP-1000 mini-computer have been transferred to a PC-based system. The initial design work for the PC database is complete. This fully searchable database in now being routinely used within the data center for editing and updating the database. Copies have been distributed to several outside user groups for comments.

CHEMICAL THERMODYNAMICS DATA CENTER

Director: Malcolm W. Chase
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. The Center provides data describing the change in the chemical properties of substances as well as bibliographic, reference and data services on thermochemistry. The Center typically provides a thermodynamic description for inorganic chemical and organic chemical containing up to two carbons. Efforts are also underway to provide estimation schemes for the ambient temperature and pressure properties of organic compounds.

The Center surveys the thermodynamic literature, extracts pertinent data, and collects this literature into a master index. This master index provides the basis for search and retrieval needs for future evaluation projects and information requests.

Thermodynamic properties of numerous alkaline earth and transition metal species are being evaluated for the JANAF Thermochemical Tables project. The initial bibliographic portion of this effort has been published. 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 nitrogen-oxygen species has been initiated.

The Center is cooperating through CODATA, with other centers located in Europe and the United States, to develop and extend an ongoing system for evaluating networks of thermodynamic information. Major accomplishments of this study are (1) determination of the (T,p) dependence of the thermodynamic properties of elemental iron, (2) the characterization of the Fe-O system as a function of temperature, pressure, and composition and (3) the analysis of the Fe++/Fe+++ system.

As part of an IUPAC cooperative effort, heat capacities of condensed phase organic species are being collected and evaluated. Also, in the area of organic thermochemistry, an ongoing program is establishing a scheme for the estimation of numeric values for 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.

Computerized versions of the JANAF Thermochemical Tables (3rd edition) and the NBS Tables of Chemical Thermodynamic Properties, both published as supplements to JPCRD, are available on the CAS/STN online service.

FLUID MIXTURES DATA CENTER

Director: Neil A. Olien
Thermophysics Division
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 OSRD and other organizations.

The computer package MIPROPS is now being distributed by OSRD 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 OSRD. Upon completion of major improvements in the transport property theoretical model, SUPERTRAPP has been delivered to OSRD for testing.

The analysis of the thermodynamic properties of methanol, benzene and toluene have 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 is in review for JPCRD. A companion set of property tables, to be published as an NBS Technical Note, is nearing completion. In addition, a critical evaluation on the properties of ethane is nearly completed, as is similar work on propane.

Conventional phase equilibrium correlations fail as the critical line is approached, and yet an accurate representation of this region and the critical line is of great industrial interest. The model and computer code under development is capable of accurately representing the critical line and can be extended well away from the critical region. A draft version of the computer code is nearly completed.

Theoretical work is being directed towards improving corresponding states and mixing rules with current emphasis on the development of a field space corresponding states formalism, improving wide range equations of state in the near critical region, and development of improved conformal solution theories for mixtures via statistical mechanical theory and computer simulation.

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 heats 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. L. Holmes (University of Ottawa), R. D. Levin (NIST), J. E. Liebman (University of Maryland Baltimore County Campus), and W. G. Mallard has been published in JPCRD. The publication gives evaluated heats of formation of approximately 8000 ions (5700 cations and 2400 anions).

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 will be ready by years end.

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.

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, the OSRD effort has principally focused on critical data evaluations, extending the studies to newly reported systems, and to data base 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
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 and the JANAF Thermochemical Tables Project. 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.

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.

Databases are assembled and used for the preparation of a variety of publications, such as data tables and bibliographies, and for online searching. Direct-dial access to the online databases is currently provided for a number of scientists in North American laboratories to the following databases: RATES, containing rate constants for 6500 reactions of inorganic radicals in aqueous solution, TTAS, containing spectral parameters for triplet-triplet absorption for 1143 organic molecules in condensed phase, and RCDCbib, the Center's bibliographic database containing over 101000 references. The online numeric databases are derived from

critical reviews prepared for publication in the JPCRD. A current-awareness service derived from RCDCbib is published biweekly and distributed to subscribers.

Critical compilations have been completed and submitted for publication in JPCRD on (1) electron transfer and energy transfer quenching rates for excited metal complexes in fluid solutions, and (2) reduction potentials for one-electron couples involving radicals in aqueous solution. A critical review of kinetic data for reactions of peroxyl radicals in solution is in progress. Currently, photophysical properties for excited states of organic molecules in polar and nonpolar condensed media are being compiled and evaluated. The properties include lifetimes, quantum yields, quenching rates, and decay times for absorption and emission. A handbook containing these properties is in preparation. The handbook will include data for a wide variety of organic molecules and will provide a basis for design of experiments involving similar molecules for which such data are not available.

THERMODYNAMIC RESEARCH CENTER

Director: K. 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 OSRD 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 on-going program for abstracting information on the properties of organic compounds. During the past year, this information has been added to the TRC Source database.

PROJECTS

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.

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.

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

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

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

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
Source 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, ^{4}He

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.

GAS PHASE NEGATIVE ION THERMOCHEMISTRY

J. E. Bartmess
University of Tennessee
Knoxville, Tennessee

A comprehensive compilation of gas phase negative ion thermochemistry is being carried out which emphasizes enthalpies of formation of anions, gas phase Bronsted acidities, electron affinities, Lewis complexation of anions, and solvation energies of anions. Evaluation and selection of the "best" values for a given anion involve analysis in terms of structure-

energy relationships, compared to a number of internally consistent overlapping reactivity scales now available.

KINETICS AND REACTION MECHANISMS OF OH RADICAL REACTIONS WITH ORGANIC COMPOUNDS

R. Atkinson
Statewide Air Pollution Research Center
University of California (Riverside)
Riverside, California

The hydroxyl (OH) radical is well recognized as a key reactive intermediate in both combustion systems and the atmosphere. Thus, degradation of organic compounds in both of these systems occurs to a large, and in many cases dominant, extent via reaction with the OH radical. An evaluation and review of the kinetics and mechanisms of the gas-phase reactions of the OH radical with organic compounds is being carried out over the entire temperature ranges for which experimental data are available. The high-temperature kinetic and mechanistic data are being compiled, tabulated and evaluated, and integrated with an earlier study by Atkinson.

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 N(x)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.

GIBBS ENERGIES OF FORMATION OF KREBS' CYCLE AND RELATED COMPOUNDS

S. L. Miller
University of California, San Diego
La Jolla, California
Source of Support: NSF

A thermodynamic network solution has been used to determine the Gibbs energies of formation of the compounds of the Krebs' cycle and compounds related to this cycle. The enthalpies of formation and the entropies have also been estimated where possible. The method uses the enzyme equilibria in the literature together with the available third law Gibbs energies of

formation. Preliminary work on this set of equilibria indicates that very accurate G_f's (±0.4 kJ) can be obtained for many of these compounds. All the available equilibrium constants and third law G_f's have been examined and used to obtain a reliable set of G, H_f and S^o for these compounds.

It is expected that useful rules can be obtained for estimating of the Gibbs energies of various reactions as soon as a basic set of accurate Gibbs energies of formation is obtained. The use of such rules will allow us to estimate the G_f's for a large number of organic compounds useful to biochemists, organic chemists, and industrial chemists.

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

Professor 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 is scattered throughout the literature in a variety of journals, books, and proceedings both foreign and domestic. This project involved the compilation and evaluation of this data with a view to providing ready access to the data itself 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 SYSTEMS

Dr. Vladimir Majer
Department of Chemistry and Biochemistry
University of Delaware
Newark, Delaware

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

Neil A. Olien
National Institute of Standards and Technology
Center of Chemical Technology
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 & 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.

DATA CENTERS

ALLOY PHASE DIAGRAM DATA CENTER

E. N. Pugh, Director
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.

CORROSION DATA CENTER

D. B. Anderson, Director
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.

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 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

A. D. Mighell, Director
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) NBS CRYSTAL DATA Distribution Package (1987); 2) International Online Search System; 3) NBS/Sandia/ICDD Database for Electron Diffraction.

The first product is NBS CRYSTAL DATA, a FORTRAN program (NBS*SEARCH), and accompanying documentation. NBS 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, the NBS/Sandia/ICDD Database for Electron Diffraction, 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 NBS 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.

PHASE DIAGRAMS FOR CERAMISTS DATA CENTER

S. Freiman, Leader
Ceramics Division, 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, and transmissivity.

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.

TRIBOLOGY INFORMATION ACTIVITY

Said Jahanmir, Leader
Ceramics Division, 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 SRD 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, 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

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. This project is jointly sponsored with the American Society of Mechanical Engineers and the Electric Power Research Institute.

BINARY PHASE DIAGRAM EVALUATION - OSRD PROJECTS

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: NIST

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, OH
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.

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.

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 ^{o}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 NBS Crystal Data ID File, which is available for on-line use.

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 will be ready for distribution in 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 NBS 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

G. B. Parker
Stanford University
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 scheme 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 reimplementation has been completed in 1988.

The major goals of the project are to demonstrate that a comprehensive materials data system can be built and 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
National Institute of Standards and Technology
Gaithersburg, Maryland
Source 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.

Journal of Physical and Chemical Reference Data, Volume 17

No. 1

Pressure and Density Series Equations of State for Steam as Derived from the Haar-Gallagher-Kell Formulation
R. A. Dobbins, K. Mohammed, and D. A. Sullivan

Absolute Cross Sections for Molecular Photoabsorption, Partial Photoionization, and Ionic Photofragmentation Processes
J. W. Gallagher, C. E. Brion, J. A. R. Samson, and P. W. Langhoff

Energy Levels of Molybdenum, MO I through MO XLII
Jack Sugar and Arlene Musgrove

Standard Chemical Thermodynamic Properties of Polycyclic Aromatic Hydrocarbons and Their Isomer Groups I. Benzene Series
Robert A. Alberty and Andrea K. Reif

No. 2

Electronic Energy Levels of Small Polyatomic Transient Molecules
Marilyn E. Jacox

Critical Review of Rate Constants for Reactions of Hydrated Electrons, Hydrogen Atoms and Hydroxyl Radicals (.OH/.O^-) in Aqueous Solution
George V. Buxton, Clive L. Greenstock, W. Phillip Helman, and Alberta B. Ross

Chemical Kinetic Data Base for Combustion Chemistry. Part 3. Propane,
Wing Tsang

No. 3

Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen $O(^3P)$ with Saturated Organic Compounds in the Gas Phase
John T. Herron

Rate Constants for Reactions of Inorganic Radicals in Aqueous Solution
P. Neta, Robert E. Huie, and Alberta B. Ross

Recommended Data on the Electron Impact Ionization of Atoms and Ions: Fluorine to Nickel
M. A. Lennon, K. L. Bell, H. B. Gilbody, J. G. Hughes, A. E. Kingston, M. J. Murray, and F. J. Smith

No. 4

Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen $O(^3P)$ with Sulfur Containing Compounds
D. L. Singleton and R. J. Cvetanovic

New International Skeleton Tables for the Thermodynamic Properties of Ordinary Water Substance
H. Sato, M. Uematsu, K. Watanabe, A. Saul, and W. Wagner

Benzene Thermophysical Properties from 279 to 900K at Pressures to 1000 Bar
Robert D. Goodwin

Estimation of the Thermodynamic Properties of Hydrocarbons at 298.15K
Eugene S. Domalski and Elizabeth D. Hearing

Wavelengths and Energy-Level Classifications of Scandium Spectra for All Stages of Ionization
V. Kaufman and J. Sugar

Atomic Weights of the Elements 1987
J. R. de Laeter

The 1986 CODATA Recommended Values of the Fundamental Physical Constants
E. Richard Cohen and Barry N. Taylor

Supplements

Gas-Phase Ion and Neutral Thermochemistry
Sharon G. Lias, John E. Bartmess, Joel F. Liebman, John L. Holmes, Rhoda D. Levin, and W. Gary Mallard

Thermodynamic and Transport Properties for Molten Salts: Correlation Equations for Critically Evaluated Density, Surface Tension, Electrical Conductance, and Viscosity Data
George J. Janz

Atomic Transition Probabilities Scandium through Manganese
G. A. Martin, J. R. Fuhr, and W. L. Wiese

Atomic Transition Probabilities Iron through Nickel
J. R. Fuhr, G. A. Martin, and W. L. Wiese

Other Publications in NIST Series

A Prototype Expert System: An Automated Advisor to Select Data Sources from Chemical Information Databases, NBSIR 88-3689
Elizabeth N. Fong, Christopher E. Dabrowski

Evaluation of Data Availability and Quality for Interaction Second Virial Coefficients of Use to the Gas Industry, NBS Tech Note 1249
Bernard J. Van Wie, Mark A. Langenberg, Wayne C. W. Chang, Kesavalu H. Kumar, and Kenneth E. Starling

Bulletin of Alloy Phase Diagrams, Vol. 9, 1988
J. F. Smith, Editor
ASM International
(Evaluations done by NBS Alloy Phase Diagram Data Center and SRD-funded projects)

Data Compilations from Other Publishers

Thermodynamic Data for Biomass Materials and Waste Components, E. S. Domalski, T. L. Jobe, Jr., T. A. Milne, 376, Amer. Soc. of Mechanical Engineers (1988)

Thermodynamic Properties of Methane in the Critical Region, D. S. Jurumov, G. A. Olchowy, J. V. Sengers, Int. J. of Thermophysics, Vol. 9, 73-84 (1987)

On Combination Rules for Molecular Van der Walls Potential Well Parameters, J. Bzowski, E. A. Mason, J. Kestin, Int. J. of Thermophysics, Vol. 9, 131-143 (1988)

Evaluation of Published Data on Ductile Initiation Fracture Toughness of Low-Alloy Structural Steels, J. of Testing and Evaluation, Vol. 16, 113-123 (1988)

Computerization of the ICDD Powder Diffraction Database Critical Review of Sets 1 to 32, Winnie Wong-Na, Camden Hubbard, Judith Stalick, E. Evans, Powder Diffraction, Vol. 3, 12-18 (1988)

Crossover from Singular to Regular Behavior of the Transport Properties of Fluids in the Critical Region, G. A. Olchowy, J. V. Sengers, Physical Review Letters, Vol. 61, 15-18 (1988)

Phase Diagrams of Binary Titanium Alloys, Joanne L. Murray, Editor, ASM International Monograph Series on Alloy Phase Diagrams

Phase Diagrams of Binary Gold Alloys, Hiroaki Okamoto and Thaddeus B. Massalski, Editors, Monograph Series on Alloy Phase Diagrams

Phase Diagrams of Binary Beryllium Alloys, Lee Tanner and Hiroaki Okamoto, Editors, ASM International Monograph Series on Alloy Phase Diagrams

Phase Diagrams of Binary Magnesium Alloys, A. A. Nayeb-Hashemi and J. B. Clark, Editors, ASM International Monograph Series on Alloy Phase Diagrams

Part 1, Phase Diagrams of Ternary Iron Alloys, V. Raghavan, Editor, Joint publication of ASM International and Indian Institute of Metals

PUBLICATIONS SCHEDULED FOR 1989

Journal of Physical and Chemical Reference Data

Compilation and Analysis of Cross Sections for K-Shell X-Ray Production by Hydrogen and Helium Ions in Elements from Beryllium to Uranium
G. Lapicki

Thermodynamic Properties of Argon from the Triple Point to 1200 K with Pressures to 1000 MPA
Richard B. Stewart and Richard T. Jacobsen

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 Kang, and Ellen Burmenko

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

Solubility of Simple Apolar Gases in Light and Heavy Water at High Temperature: A Critical Assessment of Data
Rose Crovetto and Roberto Fernandez-Prini

Thermal Conductivity of Refrigerants in a Wide Range of Temperature and Pressure
R. Krauss and K. Stephan

The Solubility of Magnetite in Water and Aqueous Solutions of Acid and Alkali
G. Bohnsack, K. Kuhnke, and H. Bohnsack

Cross Sections for Collisions of Electrons and Photons with Oxygen Molecules
Y. Itakawa, A. Ichimura, and K. Onda

Standard Electrode Potentials and Temperature Coefficients in Water at 298.15 K
Steven G. Bratsch

The Thermal Conductivity of Nitrogen and Carbon Monoxide in the Limit of Zero Density
J. Millet and W. A. Wakeham

Rate Constants for the Quenching of Excited States of Metal Complexes in Fluid Solution
Morton Z. Hoffman, Fabrizio Bolleto, and Lucia Moggi

Thermodynamic and Transport Properties of Carbohydrates and their Monophosphates: the Pentoses and Hexoses
Robert N. Goldberg and Yadu B. Tewari

Thermophysical Properties of Methane
Daniel G. Friend, James F. Ely, and Hepburn Ingham

Thermodynamic Properties of Isomeric Nitriles
Michel Bures and Cestmir Cerny

Thermodynamic Properties of Dioxygen Difluoride and Dioxygen Fluoride
John Lyman

A Fundamental Equation for Water Covering the Range from the Melting Line to 1273 K at Pressures up to 25000 MPa
A. Saul and W. Wagner

Microwave Spectral Tables II. Hydrocarbons, CH to C10H10
F. J. Lovas and R. D. Suenram

The Thermodynamics of the Krebs Cycle and Related Compounds
Stanley L. Miller

Toluene Thermophysical Properties from 178 to 800 K at Pressures to 1000 Bar
Robert D. Goodwin

Chemical Kinetic Data Base for Combustion Chemistry Part IV: Isobutane
Wing Tsang

Thermodynamic Functions and Properties of MgO and Mg_2SiO_4 at High Compression and High Temperature
Orson L. Anderson and Keshan Zou

Reduction Potentials of One-electron Couples Involving Free Radicals in Aqueous Solution
Peter Wardman

Transport Properties of Carbon Dioxide
V. Vesovic, W. A. Wakeham, G. A. Olchowy, J. V. Sengers, J.T.R. Watson, and J. Millat

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry. Supplement III
R. Atkinson, D. L. Baulch, R. A. Cox, R. F. Hampson, J. A. Keir, and J. Troe

Octanol-Water Coefficients of Simple Organic Compounds
James Sangster

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

Kinetics and Mechanisms of the Gas-Phase Reactions of the Hydroxyl Radical with Organic Compounds
Roger Atkinson

Photoemission Cross Sections for Atomic Transitions in the Extreme Ultraviolet due to Electron Collisions with Atoms and Molecules
J. M. van der Burgt

Critical Compilation of Surface Structures Determined by ion Scattering Methods
P. R. Watson

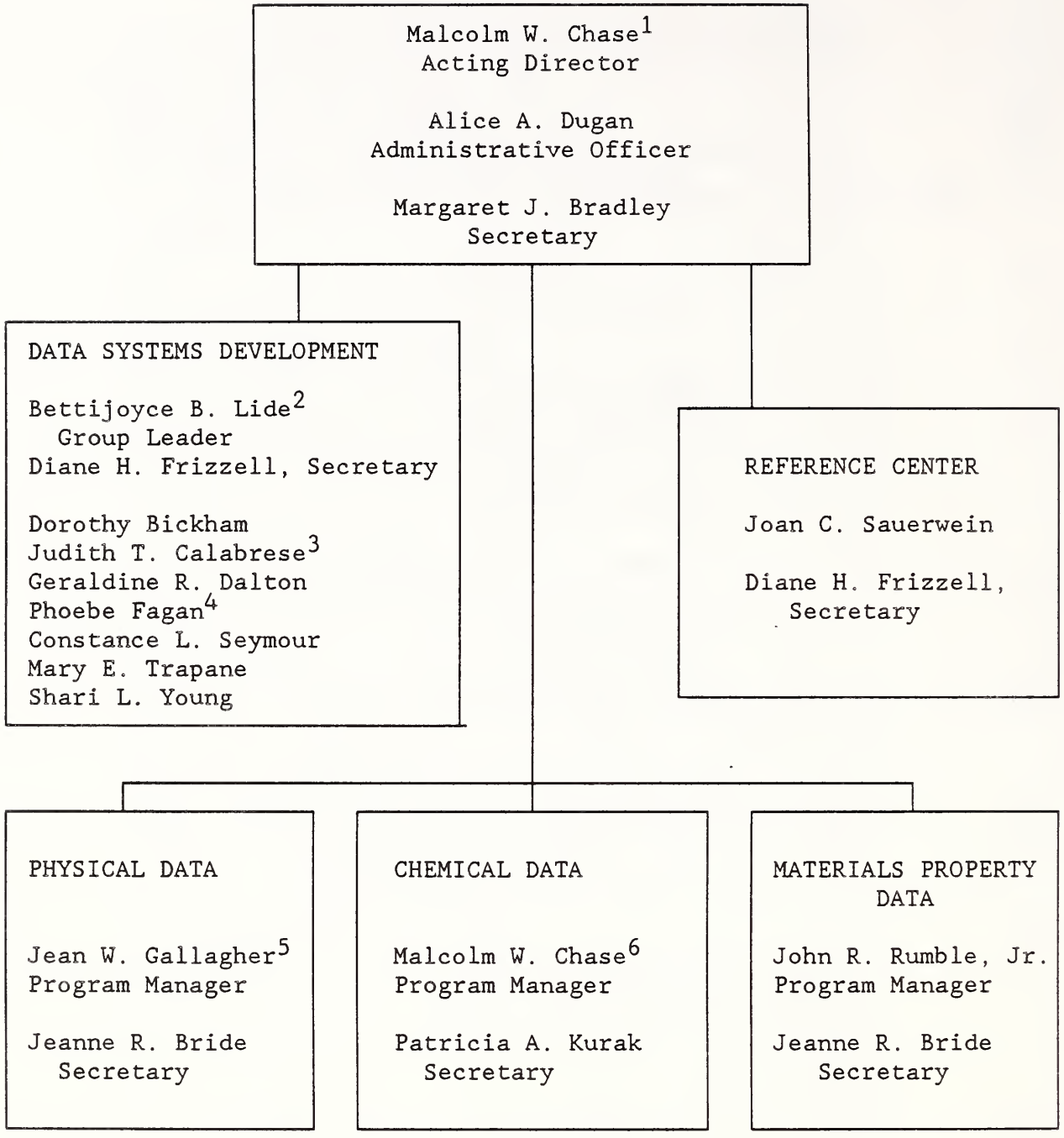
APPENDIX A

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
CAS	Chemical Abstracts Service
CBS	Center for Basic Standards, NML, NIST
CCE	Center for Chemical Engineering, NEL, NIST
CCP	Center for Chemical Physics, NML, 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 fur chemisches Apparatewesen
DIPPR	Design Institute for Physical Property Data (AIChE)
DOD	U. S. Department of Defense
DOE	U. S. Department of Energy
EMF	Electro-Motive Force
EPA	U. S. Environmental Protection Agency
ESCA	Electron Spectroscopy for Chemical Analysis
EXAFS	Extended X-ray Absorption Fine Structure
FDA	Food and Drug Administration
FIZ	Fachinformationszentrum
FY	Fiscal Year
GPE	General Purpose Equipment
GPSDC	General Purpose Scientific Document Code
GRI	Gas Research Institute
HP	Hewlett-Packard

IAPS	International Association for the Properties of Steam
ICDD	International Centre for Diffraction Data (JCPDS)
ICSU	International Council of Scientific Unions
IMSE	Institute for Materials Science and Engineering
INCRA	International Copper Research Association
IUPAC	International Union of Pure and Applied Chemistry (ICSU)
JANAF	Joint Army, Navy, Air Force (historical acronym)
JCAMP	Joint Committee on Atomic and Molecular Physical Data
JCPDS	Joint Committee on Powder Diffraction Standards
JCPDS-ICDD	JCPDS-International Centre for Diffraction Data
JILA	Joint Institute for Laboratory Astrophysics, NML, 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
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
OA	Other Agency (Funding)
OMS	Office of Measurement Services, NML, NIST
ONR	Office of Naval Research
OSRD	Office of Standard Reference Data, NML, NIST
OSTP	Office of Science and Technology Policy
PDFC	Phase Diagrams for Ceramists Data Center
PL	Public law
PMFC	Precision Measurements - Fundamental Constants
PMS	Physical Measurement Services
RCDC	Radiation Chemistry Data Center
SAE	Society of Automotive Engineers
SPE	Society of Plastics Engineers
SRD	Standard Reference Data
SRM	Standard Reference Material
STRS	Scientific and Technical Research and Services (appropriated NIST funds)
TRAPP	Thermophysical Properties of Hydrocarbon Mixtures Database
UNESCO	United Nations Educational, Scientific, and Cultural Organization
USGS	United States Geological Survey

OFFICE OF STANDARD REFERENCE DATA



[1]David R. Lide retired as Director in October 1988
[2]Also on detail to NML Office since June 1988.
[3]Oversees work of Bedford Group
[4]Oversees work of Data Systems Group
[5]Succeeded Sharon G. Lias on September 1, 1988
[6]Succeeded Howard J. White, Jr., who retired on January 3, 1988

STAFF OF THE OFFICE OF STANDARD REFERENCE DATA - November 1988

Acting Director - Dr. Malcolm W. Chase
Secretary, Mrs. Margaret J. Bradley
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 Gallagher
Secretary, Mrs. Jeanne R. Bride
Telephone: (301) 975-2204

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

Program Manager - Dr. Malcolm W. Chase
Secretary, Mrs. Patricia A. Kurak
Telephone: (301) 975-2205

Management of Chemical 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 Data Program - mechanical properties, corrosion, phase diagrams

Reference Center - Mrs. Joan C. Sauerwein
Telephone: (301) 975-2208
Secretary, Mrs. Diane H. Frizzell

Coordination of OSRD publication process; response to data inquiries from the public; maintenance of NSRDS collection of main NIST Library and OSRD Reference Center holdings; distribution of databases; exhibits

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

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

As Executive Secretary of the International Association for the Properties of Steam (IAPS) and a member of the U.S. National Committee for the Properties of Steam (the U.S. member of IAPS), as a member of several committess of DIPPR, and as a corresponding member of the CODATA Task Group on Chemical Thermodynamic Tables, is involved in the management, direction and programs of these organizations which include cooperative projects in which NIST scientists participate and projects which produce databases marketed by OSRD.

Data Systems Development Group
Group Manager - Mrs. Bettijoyce B. Molino
Secretary, Mrs. Diane H. Frizzell
Telephone (301) 975-2218

Management of OSRD activities related to data center automation, development of online data storage and retrieval techniques, computer typesetting techniques, computerized databases

Mrs. Dorothy Bickham
Telephone (301) 975-2524

Software development and application for data automation and dissemination.

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

Computer typesetting of NSRDS publications via the Bedford Composition System; system control and preparation of user interfaces to the composition system.

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

Development of software for data automation of data center activities; preparation of databases for distribution

Mrs. Phoebe Fagan
Telephone: (301) 975-2213

System manager and consultant for SRD Computer Facilities; programming for data automation and dissemination

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

Processing and pagination both internally of files received from outside data centers through composition system; reproduction and inventory control of NIST Standard Reference Database Series

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

Assistance in programming for data automation and dissemination; processing of files for typesetting.

Miss Shari L. Young
Telephone: (301) 975-2216

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

APPENDIX D

PUBLICATIONS BY OSRD STAFF

"Thermodynamic Properties of the Elements," M. W. Chase, Proceedings of a symposium sponsored by the ASM-MSD Alloy Phase Diagram Data Committee, held at the Fall Meeting of the Metallurgical Society in Cincinnati, Ohio, USA October 12-13, 1987.

"Thermodynamic Properties of Halides, Hydrides, and Deuterides of Cobalt, Iron, and Nickel, I. Literature Citations," Cynthia R. Jackson and Malcolm W. Chase, NBS Technical Note 1244, December 1987.

"Thermodynamic Properties of the Alkaline Earth Metal Hydroxides (MOH), I. Literature Citations," Malcolm W. Chase, NBS Technical Note 1243, December 1987.

"The NBS/EPA Data Base of Evaluated Electron Ionization Mass Spectra," W. L. Budde, S. G. Lias, S. R. Heller, and G. W. A. Milne, The Wiley/NBS Registry of Mass Spectral Data, Publishers: John Wiley & Sons, Inc., in press.

"Gas-phase Ion 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, Suppl. No. 1 (1988).

"Concerning the Formation and the Reaction Kinetics of Phenylium Ions," P. Ausloos, S. G. Lias, T. J. Buckley, and E. E. Rogers, Int. J. Mass Spectrom. Ion Proc., submitted.

"Numeric Databases for Use in Analytical Chemistry," S. G. Lias, NIST J. Res., submitted.

"Reactions of $C_5H_5^+$ and $C_5H_3^+$ Ions with Acetylene and Diacetylene," F. Ozturk, M. Moini, F. W. Brill, J. R. Eyler, T. J. Buckley, S. G. Lias, and P. J. Ausloos, J. Phys. Chem., submitted.

"Materials Data Banks in the United States," David R. Lide, Metaux Corrosion Industrie, Vol. 63, 162-166 (May-June 1988).

"Scientific Data and the Information Revolution," David R. Lide, Newsletter of the Japan Society of Information and Knowledge, submitted.

APPENDIX E

TALKS AND PRESENTATIONS BY OSRD STAFF

Malcolm W. Chase

"Numeric databases in chemical thermodynamics at the U.S. National Bureau of Standards," ACA Annual Meeting, Philadelphia, Pennsylvania, June 1988.

"Thermodynamic Databases for Inorganic Chemicals," Workshop on SRD Chemical Databases, National Bureau of Standards, Gaithersburg, Maryland, July 1988.

"Thermodynamic Properties of the Elements," 1987 TMS Fall Meeting, Physical Metallurgy and Materials, Cincinnati, Ohio, October 1987.

Phoebe Fagan

"National Standard Reference Database Series," ACS-CINF, Royal York Hotel, Toronto, Canada, June 1988.

"Fortran from RTE to HPUX," Interex Conference, Orlando, Florida, August 1988.

"Database Demonstration - Session Chairman," Thermophysics Symposium, NBS, June 1988.

"Design & Optimization Series - Session Chairman," Interex Conference, Orlando, Florida, August 1988.

Jean W. Gallagher

"Atomic and Molecular Data Needed for Astrophysics," Jean W. Gallagher, 11th International CODATA Conference, Karlsruhe, FRG, September 26-29, 1988.

Sharon G. Lias

"Structures of Ions," Washington Area Mass Spectrometry Interest Group, October 5, 1987.

"Gas-phase Ion and Neutral Thermochemistry," East Coast ICR and Ion/Molecule Reactions Symposium, University of Delaware, October 17, 1987.

"Databases for Analytical Chemistry," Symposium on "Scientific Numerical Databases - Present and Future," American Chemical Society Meeting, Toronto, Canada, June 7, 1988.

"Numeric Databases for Chemical Analysis," Workshop on "Role of Numeric Databases in Materials and Biological Sciences," American Crystallography Association Meeting, Philadelphia, PA, June 26, 1988.

"The NBS/EPA/MSDC Mass Spectral Database," Workshop on "Qualities Desirable in Mass Spectral Data Collections," 36th American Society for Mass Spectrometer Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, June 9, 1988.

"An Improved Version of the NBS/EPA/MSDC Mass Spectral Data Base, Evaluation of the Quality Index, and Data Base Software for an MS-DOS Personal Computer," by S. E. Stein, S. G. Lias, W. L. Budde, D. T. Terwilliger, and A. L. Behbehani, 36th American Society for Mass Spectrometer Conference on Mass Spectrometry and Allied Topics, San Francisco, CA, June 10, 1988.

"The NBS/EPA/MSDC Mass Spectral Database," Workshop on "Collection and Evaluation of Reference Mass Spectra," 11th International Mass Spectrometry Conference, Bordeaux, France, September 1, 1988.

"Structures and Reaction Kinetics of $C_6H_5^+$ Ions," 11th International Mass Spectrometry Conference, Bordeaux, France, September 1, 1988.

David R. Lide

"Scientific Data and the Information Revolution," 2nd International Conference on Information and Knowledge, Tokyo, Japan, November 1987.

"Materials Data Banks in the United States", CODATA/France Workshop on Materials Data Banks, Bordeaux, France, November 26, 1987.

"Numerical Data in Science and Technology, ICSU General Committee Meeting, November 1987.

"Report on Copyright in the U.S.A.," Legal Issues Group, International Council for Scientific and Technical Information, Rennes, France, May 1988.

"Goals and Structure of CODATA," Third Chemical Congress of North America, Toronto, Canada, June 1988.

"Assuring Reliable Data for Science and Technology," Third Chemical Congress of North America, Toronto, Canada, June 7, 1988.

"Copyright Issues Affecting Scientific Numerical Databases," 11th International CODATA Conference, Karlsruhe, FRG, September 1988.

Bettijoyce B. Molino

"Computerized Dissemination of Numeric Data for Chemists" - Session Chairman - Third North American Chemical Conference, Toronto, Canada, June 1988.

"National Standard Reference Database Series," Third North American Chemical Conference, Toronto, Canada, June 1988.

"The CODATA Referral Database," Third North American Chemical Conference,

Toronto, Canada, June 1988.

"The ICSTI Directory of Numeric Machine Readable Databases," Third North American Chemical Conference, Toronto, Canada, June 1988.

"The ICSTI Directory of Numeric Machine Readable Databases", 11th International CODATA Conference.

"Data for Geo and Space Sciences" - Session Chairman - 11th International CODATA Conference.

John R. Rumble

"Computer Technology Overview," Second Conference on Computerization of Welding Information, New Orleans, LA, October 1988.

"Materials Property Data in Machine-Readable Form - The Need and Challenges," Workshop on Materials Property and Design Data Needs in Canada, Toronto, Canada, October 1988.

"Databases in Chemistry, Physics, and Materials - What's Out There and Why," Special Libraries Association, Denver, CO, June 1988.

"Needs for Materials Data Activities," Numerical Data Advisory Board Subpanel on Data Needs for High Tech Materials, Washington, DC, May 1988.

"Materials Databases," International Workshop on Fatigue Databases, Boulder, CO, January 1988.

"Materials Databases - How to Build Them," Building Thermal Envelope Coordinating Council, Washington, DC, June 1988.

EXHIBITS BY OSRD STAFF

The Pittsburgh Conference and Exposition on Analytical Chemistry and Applied Spectroscopy - New Orleans, LA - February 22-25, 1988

The Third Chemical Congress of North America - Toronto, Ontario, Canada- June 5-8, 1988

World Materials Congress - 1988 Materials, Applications & Services Exposition - McCormick Place, Chicago, IL - September 27-29, 1988

APPENDIX F

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Dorothy Bickham

Hewlett Packard Users Group

Judith T. Calabrese

Bedford Composition System Users Group

Malcolm W. Chase

CODATA Task Group on Chemical Thermodynamic Tables (Chairman)

Engineering Sciences Data Unit Ltd. (Corresponding Member)

ASTM E27 Hazard Potential of Chemicals (Vice Chairman)

ASTM E49 Computerization of Material Property Data

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

ACS Task Force on Scientific Data

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

Workshop on Chemical Processes and Products in Severe Reactor Accidents

Geraldine R. Dalton

Hewlett Packard Users Group (Newsletter Editor)

Phoebe Fagan

Hewlett Packard Users Group (Chairman)

SIGUNIX of Hewlett Packard International Technical Users

Sharon G. Lias

Member, Editorial Board of the series, "Molecular Structure and Energetics," VCH Publishers, Inc.

Member, Editorial Board of the NBS Journal of Research

Member, American Institute of Physics Subcommittee on Numerical Data Bases

Member, Executive Council of the Joint Committee on Atomic and Molecular Physical Data

Member, Advisory Committee for the Clearinghouse for Digital Infrared Spectra

Member, Organizing Committee, NATO Advanced Study Institute on "Fundamentals of Ion Chemistry"

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

Bettijoyce B. Molino

NIST User Committee for Scientific Computing

NIST Personal Computer Advisory Committee

NIST National Measurement Laboratory EEO Advisory Panel

NIST National Measurement Laboratory Performance Standards Review Board

ACS Division of Chemical Information (Treasurer)

ACS Division of Chemical Information, Awards Committee

ACS Committee on Publications, Associate Member

ACS Software Advisory Board

CODATA Task Group on a Referral Database (Secretary)

Scientific Program Committee of the 11th International CODATA Conference

ICSTI Numerical Data Group

John Rumble

ASTM Committee E-49 Computerized Materials Data (Chairman)

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 Group on Factual Materials Data Banks (Head)

Task Force on Materials Database Development, Federal Cabinet Council on Science, Engineering and Technology Committee on Computer Research and Applications (Member)

Alloy Phase Diagram International Commission - CODATA Representative

ASM International - Metals Information Committee

Interagency Panel on Materials Data - Working Group (Chairman)

ASTM Committee E-42 Surface Analysis

VAMAS Workshop on Standards for Factual Materials Databanks, Petten, Netherlands, November 1988 (Cochairman)

International Workshop on Fatigue Databases, Boulder, CO, January 1988 (Cochairman)

Chemical Abstracts Service Research Conference, Columbus, OH, October 1988 (Organizing Committee)

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

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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

82 STAT. 340

DEFINITIONS

SEC. 2. For the purposes of this Act—

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

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

Collection and publication of standard reference data.

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

Standards, etc. Publication in Federal Register.

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

Sale of reference data. Cost recovery.

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

31 Stat. 1449; Ante, p. 34.

U. S. copyright and renewal rights.

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

61 Stat. 655; 76 Stat. 446.

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

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

Appropriation.

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

Short title.

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

Approved July 11, 1968.

LEGISLATIVE HISTORY:

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

GPO 98-139

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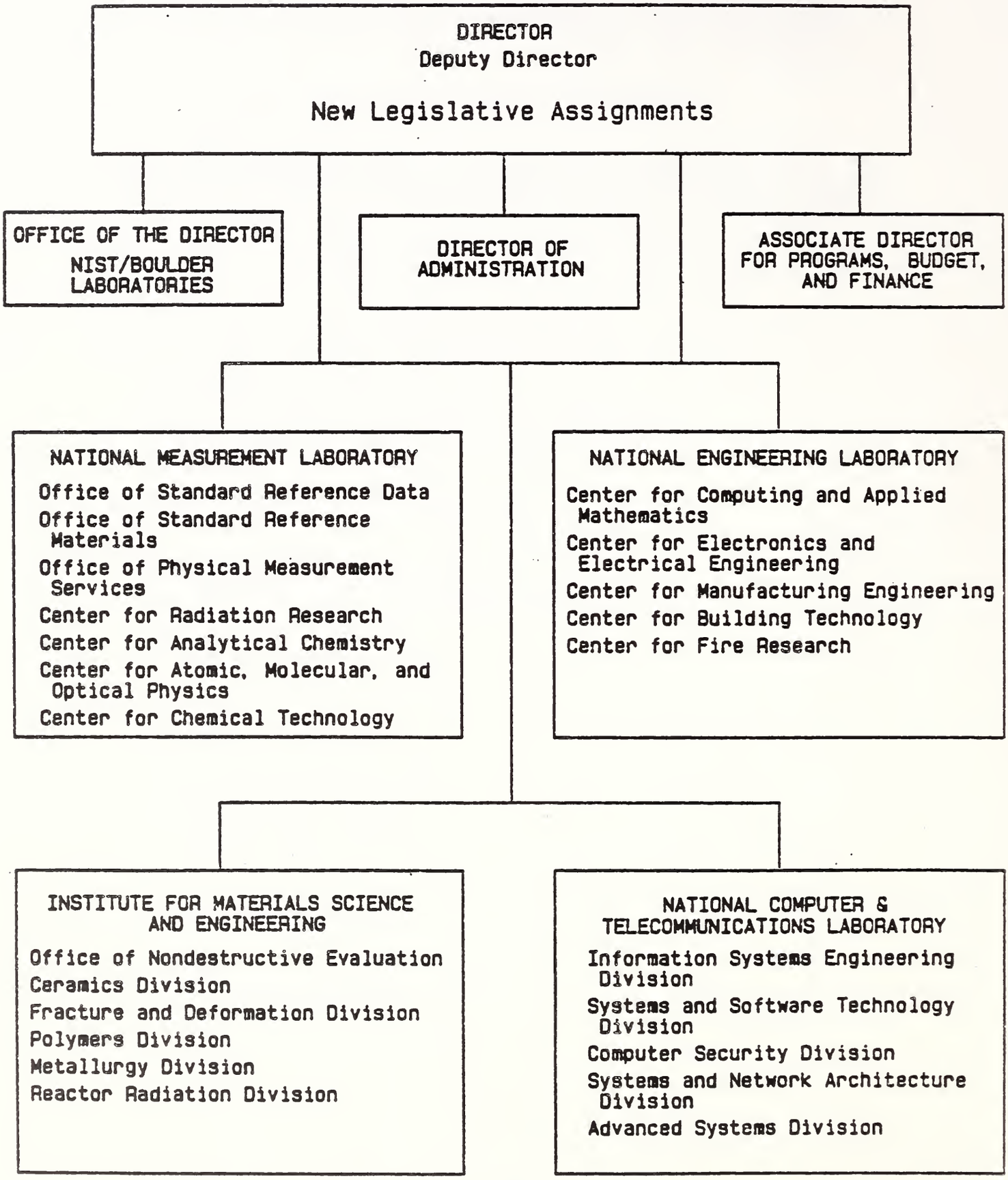
*The Office of Standard Reference Data is not involved at the present time in the administration or funding of these data centers but assists in making their outputs and services known to the scientific community.

NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY

Interim (unofficial) organization



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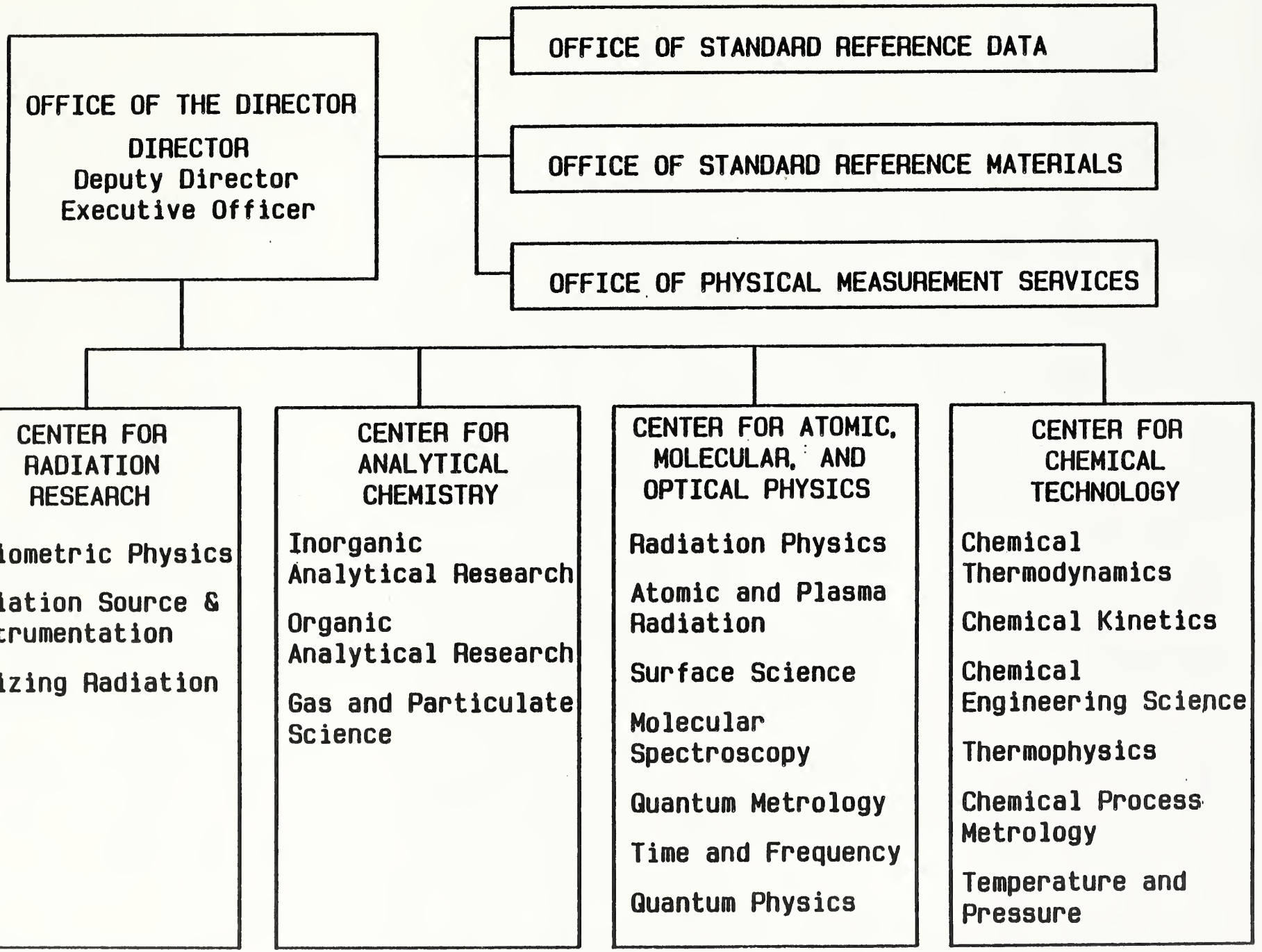

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10. SUPPLEMENTARY NOTES

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

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

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

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1988.

12. KEY WORDS (Six to twelve 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 1988.

13. AVAILABILITY

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