NBSIR 87-3526

Technical Activities 1986

Office of Standard Reference Data

February 1987

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards

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February 1987

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ABSTRACT

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

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1986.

Key words: chemical data; data compilation; evaluated data; materials properties data; numerical database; physical data; standard reference data; technical activities 1986.

TABLE OF CONTENTS

APPENDICES

INTRODUCTION

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

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

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

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

*See Appendix G

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

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

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 Bureau of Standards by the American Institute of Physics and the American Chemical Society.

NSRDS-NBS Series and other NBS 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 1986

Series	Pages Published	Titles Published
JPCRD, Vol. 15	1445	22
Data Compilations from other publishers	400	
Other Publications in NBS Series	517	3
Bibliographies and indexes from other publishers	910	2
Totals	3272	27

Subscribers to JPCRD

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

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

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

*Projected to end of year

PHYSICAL DATA

S. G. Lias, Program Manager (April 1, 1986 - September 30, 1986)
S. P. Fivozinsky, Program Manager (October 1, 1985 - March 31, 1986)

The Physical Data Program comprises data centers and projects handling data from the disciplines of atomic and molecular physics. The Physical Data Program also includes the Spectral Data Project, which deals with the administration and development of spectral databases for use in analytical chemistry.

The following data centers are associated with the Physical Data Program.

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

The projects which are currently active in the Physical Data Program are as follows:

- Spectral Data Project
- Spectroscopic Properties of Excited Electronic States of Small Polyatomic Transient Molecules
- Soft X-Ray Interactions with Matter (Photon and Charged Particle Data Center Special Project)
- Atomic Transition Probabilities for Energy Research (Atomic Transition Probabilities Data Center Special Project)
- Critical Compilations and Reviews of Data Describing the Electron Impact Excitation of Atoms and Atomic Ions (Atomic Collision Cross Sections Data Center Special Project)

The Spectral Data Project, described in detail below, includes several related tasks having to do with the administration and generation of databases for use in analytical chemistry. The second listed project is a compilation undertaken by an NBS senior scientist. The other three projects are special activities carried out within data centers of the Physical Data Program, as indicated.

Recent activities and accomplishments within the Physical Data Program are described below.

Spectral Data Project

During the past year, considerable attention has been given to the Spectral Data Project. The nucleus of the project is the NBS/EPA Mass Spectral Database which is distributed in machine-readable form by the Office of Standard Reference Data. This database, consisting of 43,000 evaluated electron ionization mass spectra, was developed during the past 20 years through the cooperative efforts of several government agencies (notably EPA and NIH) and the Mass Spectrometry Data Center of the Royal Society of Chemistry (England). At the present time, the project is jointly administered by NBS and the Office of Research and Development of the Environmental

Protection Agency. Under an agreement signed last year, the EPA carries out acceptance and insertion of new spectra, applies standard evaluation procedures to the spectra, and generates periodic updates of the database. The Office of Standard Reference Data sponsors the collection of new spectra, arranges for dissemination of printed and computer-readable versions of the file, and manages the revenues resulting from lease or sale of the database and the reinvestment of those funds in the further development of the system. The 1985 NBS/EPA agreement also specified that attention would be given to the possible joint development of a database of infrared spectra.

Meeting of the Advisory Committee on Spectral Data. Last year, as part of the NBS/EPA agreement, an Advisory Committee for the Spectral Data Project was set up. This committee consists of five well-known scientists active in the fields of mass spectrometry and/or infrared spectroscopy. The members are:

Dr. Charles Anderson (Nicolet Analytical Institute)
Dr. Robert Finnigan (Finnigan Instruments)
Dr. Jeanette Grasselli (Standard Oil of Ohio)
Dr. Milton Levenberg (Abbott Laboratories)
Dr. Charles Wilkins (University of California-Riverside)

The first meeting of the Advisory Committee, held in Chicago on February 7, 1986, featured presentations by Dr. Sherman Fivozinsky (OSRD) and Dr. William Budde (EPA). The Committee recommendations were: (1) a high priority should be given to maintaining/improving the quality of spectra in the database; (2) steps should be taken to increase the size of the database; (3) NBS and EPA should explore the feasibility/advisability of expanding the Spectra Data Project to include other types of spectra, such as IR spectra and chemical ionization mass spectra. The paragraphs below will describe the progress which has been made since February in implementing these recommendations.

Improvements in Quality - The 1986 Update of the Database. Budde (EPA) and members of his staff have modified the evaluation procedure for mass spectra in the database. The Quality Index is a numerical measure of the quality of an individual spectrum based on an algorithm that automatically examines certain features of the data (number of ions, sample purity, etc.). During the past year, the EPA scientists revised the standard algorithm to make the evaluation more sensitive to certain common errors found in spectra, such as the presence of saturated peaks.

When multiple spectra of the same compound are included in the database archive, only that spectrum with the highest Quality Index value is actually included in the distributed version. As a result of the revisions in the evaluation algorithm, the entire archive of more than 70,000 spectra was re-evaluated, and approximately 2,000 spectra in the database were replaced by spectra of better quality from the archive. Some 300 spectra which had been found to be mislabeled were corrected or eliminated. Seven-hundred new spectra were added to the database. The updated version of the database is ready to be released.

Increasing the Size of the Database of Electron Ionization Spectra. Three mechanisms have been put in place for obtaining new spectra for the mass spectral database. (1) The archive contains approximately 9,000 spectra which could not be used in the evaluated database because the relevant chemical

compounds were identified by nonstandard names, so that Chemical Abstracts Registry Numbers could not be assigned. An organic chemist with a specialized knowledge of organic nomenclature has been hired by OSRD on a contract basis to examine the "nonstandard" names, and to assign correct names and Registry Numbers. At this writing, 2000 spectra from this group have been retrieved for the database, and work is continuing. (2) A new Memorandum of Understanding between NBS and the Royal Society of Chemistry (England) has been signed; under this agreement, the Mass Spectrometry Data Center in Nottingham will resume collecting mass spectra from the literature for OSRD. At the present time, they have on hand 3786 spectra to be sent to EPA to be evaluated for the database. (3) Letters were sent to the directors of 45 industrial laboratories asking for contributions of spectra from their databases for inclusion in the NBS database. To date, 15 industrial laboratories have agreed to contribute spectra. Because of the positive response to the initial request, letters are being sent to the directors of an additional 20 industrial laboratories known to be active in the use of mass spectrometry.

The net increase in the size of the archive of mass spectra to be expected during the next year from the operation of the first two of these mechanisms will be more than 12,000 spectra, and it is anticipated that at least 10,000 spectra will eventually be acquired from the 15 industrial laboratories which have already agreed to participate.

OSRD has also initiated conversations with Dr. F. W. McLafferty of Cornell University, a leading mass spectrometrist who is also actively engaged in building a database of mass spectra. The possibility of collaborative efforts is being explored.

Expansion of the Spectral Database Project.

Chemical Ionization Mass Spectra. Several scientists who have been active in the development and use of the analytical technique known as Chemical Ionization (CI) were consulted about the need for a database of CI spectra and the feasibility of developing such a database. The consensus was that at the present time, the conditions under which CI spectra are run are not sufficiently standardized to permit the evaluation of such a database. However, there is also general agreement that there is a need to evaluate and standardize operating conditions so that a comparison library of CI spectra could be used to identify unknown compounds. Scientists, particularly the leadership of the ASTM Committee E-14, are interested in working with OSRD to organize an evaluation effort which could lead to the recommendation of standard operating conditions and, eventually, to the building of a database of evaluated CI spectra.

Infrared Spectra. The NBS/EPA agreement specified that the two agencies will investigate the need for and feasibility of development of a database of infrared spectra. At the present time, details of existing IR databases are being analyzed in order to assess the needs of the user community.

NMR Databases. Dr. Charles Wilkins of the Advisory Committee on Spectral Databases has suggested that OSRD investigate the needs for databases of NMR spectra.

Publication of New Hard Copy of Mass Spectral Database. The mass spectral database appeared in book form in 1978. The original four volumes were updated with a two-volume supplement which appeared in 1982. These books, published by the Government Printing Office, are now out-of-print, and there is considerable demand from users for a hard-copy version of the current (1986) update of the database. Two publishers have expressed an interest in publishing the books. A Request for Proposal (RFP) describing a proposed new publication has been prepared and is being processed.

Project on Spectroscopic Properties of Excited Electronic States of Small Polyatomic Transient Molecules. This is a two year project undertaken by Dr. Marilyn Jacox of the Center for Chemical Physics. The details of the project are described elsewhere. Recent accomplishments are:

A database of ground-state vibrational energy levels of transient molecules has been created and is being maintained up-to-date.

A database of electronic spectral data for polyatomic transient molecules possessing from 3 to 6 atoms has been initiated.

Data Centers

Publications, reports, and databases completed or in progress during the past year from the Data Centers of the Physical Data Program are listed below.

Atomic Collision Cross Section Data Center:

"Absolute Cross Sections for Molecular Partial Photoionization and Photofragmentation Processes," to be submitted for publication in FY 87.

"A Review of Optical Excitation Functions for Atoms and Atomic Ions," in progress.

"Collisional Alignment and Orientation of Atomic Outer Shells. I. Direct Excitation by Electron and Ion Impact," Physics Reports, submitted.

Atomic Energy Levels Data Center

Critical Compilation of Forbidden Lines in the Spectra of Atoms and Ions, Beryllium through Molybdenum, JPCRD 15, 321 (1986).

Energy Levels for the Iron Group Elements, JPCRD 14, Suppl. 2 (1985).

Atomic Transition Probabilities Data Center

"Spectroscopic Data for Iron," Vol. IV of series "Atomic Data for Fusion," ORNL, 1986.

"Spectroscopic Data for Ti and Ni Ions," in preparation.

Fundamental Constants Data Center

"Impact of Quantized Hall Resistance on SI Electrical Units and Fundamental Constants," Metrologia 21, 37 (1985).

"New Results from Previously Reported NBS Fundamental Constant Determinations," J. Res., Natl. Bur. Stand. 90, 91 (1985).

"Electrical Units, Fundamental Constants, and the 1983 Least-Squares Adjustment," IEEE Trans. Instrum. Meas. IM-34, 155 (1985)

Recommended Consistent Values of the Fundamental Physical Constants, 1986, Report of the CODATA Task Group on Fundamental Physical Constants," in progress.

"The 1986 Least Squares Adjustment of the Fundamental Constants," to be submitted for publication in JPCRD in FY 87.

Molecular Spectra Data Center

"Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions - 1985 Revision," JPCRD 15, 251 (1986).

"Microwave Spectral Tables. Part III - Hydrocarbons," to be submitted to JPCRD.

Photon and Charged Particle Data Center

"XGAM," a database of X-ray and gamma ray attenuation coefficients as well as scattering, photoabsorption and pair-production cross sections for any element, compound or mixture, completed during the past year, now being distributed on magnetic tape. The photon cross section database was also restructured and streamlined for use with a microcomputer.

"EPSTAR," a database of electron and positron stopping powers, was completed and is now being distributed on magnetic tape.

"Bremsstrahlung Spectra for Electron Interactions with Screened Atomic Nucleii and Orbital Electrons," Nuclear Instruments and Methods, B12, 95 (1985)

"Bremsstrahlung Energy Spectra for Electrons with Kinetic Energy from 1 keV to 10 GeV Incident on Screened Nuclei and Orbital Electrons of Neutral Atoms with Z = 1 to 100," Atomic Data and Nuclear Data Tables, in press.

H. J. White, Jr. Program Manager

The program in chemical data is developed in three primary areas: chemical thermodynamics, thermophysical properties, and chemical kinetics. Chemical thermodynamics includes those thermodynamic properties needed to quantitatively describe chemical equilibria over a range of ambient conditions. Thermophysical properties include transport and electrical properties a well as those thermodynamic properties needed to describe the equilibrium behavior of substances as functions of temperature and pressure. Activities in chemical kinetics include gas-phase homogenous kinetics, gas-phase reactions involving ions, and radiation and photochemistry in solution.

Taken in conjunction with the program on materials properties, these areas cover a wide range of scientific and industrial needs although there are important gaps, for example, heterogeneous kinetics. The fit of the program to industrial needs can be seen from some of the cooperative programs with industrial organizations such as DIPPR and IAPS which will be discussed in more detail further on.

The program is carried out through a series of data centers and project grants. A project grant covers a limited time and involves one or a few reference-data products. The operators of a data center accept responsibility for providing reference data in a given field and establish and maintain reference files in the field as well as produce reference-data products. By its nature a data center is a longer term operation than a project grant and is capable of producing more varied and sophisticated products and services.

Two distinctive characteristics of the activities making up the program in chemical data will be mentioned: they are heavily involved in automation and in cooperative projects with other organizations. This is particularly true of the data centers.

Automation covers three areas: database management, automated transfer of data between data centers, and automated products. The nature of a data center's activity makes database management a central function, a function which is complicated by the nature of chemical nomenclature with its multiple synonyms and use of global formulae, line formulae, etc. In addition, it is desirable to be able to index by chemical reaction as well as substance. Transfer of automated products via tape, cassette, or diskette is used routinely. More direct methods involving accessing data files on another computer and down-loading them to the home computer are growing. Automated products range from using computer files or tapes to prepare camera-ready hard copy to readable tapes, interactive tape programs and interactive PC programs.

Cooperative projects are attractive and important for various reasons. First, users prefer a single definitive source for reference data. Such a source minimizes disputes about the quality of alternative sources and simplifies search and retrieval for the users. Second, the resources available for the production of reference data the world over are so limited that it is important that they be used efficiently and that duplication of effort be minimized. It is also necessary that the highest quality be maintained. Although some users' needs may be satisfied by data of lesser quality, a

substantial fraction of the users will require the highest quality available. The level of quality available changes with time as new measurements are made and better understanding of the underlying science improves evaluation techniques. As a result, the best way to obtain authoritative reference data is through the combined efforts of a number of recognized experts in the field or fields involved. The cooperation may take place through the activities of international scientific or technical groups or through national disciplinary or trade associations.

Brief highlights for each major program area follow. They are not exhaustive and do not list all on-going activities or papers prepared for publication. Published papers are listed elsewhere.

Chemical Thermodynamics

Chemical thermodynamic data are generated by the Chemical Thermodynamic Data Center, the Aqueous Electrolyte Data Center and the Ion Kinetics and Energetics Data Center at NBS, the Thermodynamic Research Center at Texas A&M University and by grant projects at MIT, and the Universities of Delaware, and California at San Diego. Cooperative efforts are widespread and include interactions with the National Center for Thermodynamic Data on Minerals, a U.S. Geological Survey data center in Reston, VA, and data centers in Harwell, U.K., Grenoble, France, and Moscow, USSR, through the CODATA Task Group on Chemical Thermodynamic Tables, and with the Design Institute for Physical Properties Data of the AIChE (DIPPR).

A major product in this area is the first volume of the CODATA Chemical Thermodynamic Tables. This represents, simultaneously, the first publication of a new generation of chemical thermodynamic tables and a report to the thermodynamics community by the CODATA Task Group. The tables differ from previous tables in a variety of ways. They provide thermochemical properties for formation of individual substances and binary systems as well as thermal functions for them over a wide range of temperature and composition in a thermodynamically consistent way. The total range of coverage is greater than in any one previous table. Because of a carefully controlled systematic approach and extensive use of automated procedures, they have been produced in a decentralized way by groups in four countries. Finally, they can be updated and extended in a thermodynamically consistent way. Technical difficulties in doing these latter tasks for previous tables meant that, for practical purposes, workers had to start again from the beginning. In the future it should prove possible for groups which are evaluating data for different classes of substances for various reasons to use their efforts to make contributions to the CODATA Tables which would serve as a comprehensive international set of reference values. In this way it should prove possible to build up consistent tables containing a large number of compounds much more rapidly than has been the case in the past and to expand and update them systematically.

The first volume contains data on a number of compounds of calcium and magnesium, an alloy, a high-temperature mixture, and an aqueous solution. Currently the task group is working on iron compounds, again with alloys, high-temperature mixtures, and aqueous solutions included. In addition to the work of the members of the task group, contributions have been received from the National Center for Thermodynamic Data on Minerals, and it may be that the Scientific Group Thermodata Europe will also participate in the work.

A related task is the preparation of the CODATA Key Values for Thermodynamics for publication. The key values are formation properties for a set of key thermodynamic substances which have been used extensively in reactions that determine the thermodynamic formation properties of other substances. As such, the data for these substances are of unusual importance, and publication of reference values for them can form the basis for many other compilations. For example, the CODATA Tables are based on them.

A third major publication is the third edition of the JANAF Tables which will be made available in printed and automated forms. These well known tables are extensively used in science and industry. In this connection it is a pleasure to point out that Dr. Malcolm Chase, the director of the JANAF Thermochemical Data Project, has joined the Chemical Thermodynamic Data Center and intends to carry on the JANAF work in the center.

Another major effort in this area is also drawing to a close. This involves compounds containing up to four carbon atoms as well as hydrogen and oxygen. Properties for which data will be given are condensed phase and ideal-gas thermal functions, and formation properties, although the experimental data are not available to allow each type of data for every compound.

A joint effort involving the Aqueous Electrolyte Data Center, the University of Delaware, and now DIPPR as well, is concerned with providing accurate reference data for the properties of aqueous electrolyte solutions over an extended range of temperatures. These data are needed for the understanding and control of corrosion and pollution in the chemical, petroleum, and power industries. In this last category they are of great interest to IAPS. Tables to 373 K have already been published; extension to higher temperatures involves consideration of pressure as well as concentration and temperature. Consideration of the behavior of aqueous solutions in the critical region is being carried out in the Polar Fluids Project.

The data centers on chemical thermodynamics, aqueous electrolytes, ion energetics, and chemical kinetics cooperate in the development of automated programs useful to all four centers. Two such systems have been completed recently. One is a general search and retrieval system for indexed material containing text and/or tabular material. This is an online system available through terminals to all centers. A common bibliographic system has also been placed online and is being tested.

Thermophysical Properties

Thermophysical properties data are provided by the Fluid Mixtures Data Center and the Polar Fluids Project at NBS, the Design Institute for Physical Properties Data of the AIChE, and grant projects at Brown University (2), the University of Maryland, the University of Idaho, and the University of Oklahoma.

A new interactive automated product, to be made available in tape form for mainframe computers and diskette for micro computers is called MIPROPS. It provides thermodynamic and thermophysical properties for 12 fluids. It supersedes and replaces NBS Data Bases 5 and 6. The fluids covered are

argon, ethylene, parahydrozen, nitrogen, nitrogen trifluoride, oxygen, helium, methane, ethane, propane, isobutane, and butane. The data for the first six fluids have already been published, a publication for the remainder is in process. Tables based on the formulations used for argon, oxygen, nitrogen, helium, and hydrogen have been supplied to the Compressed Gas Association for use in custody-transfer calculations. Tables based on the same formulation have also been provided to OIML where they are under consideration as international standards.

A monograph on ethylene is to be published in the IUPAC International Thermodynamic Tables of the Fluid State series. The formulations on which this monograph is based were prepared as part of the Joint Industry Government Ethylene Project. The project and the monograph involved extensive contributions from the NBS laboratories at Gaithersburg and Boulder and by OSRD. The formulations provide a marked improvement over currently available formulations, and tables and should become widely used.

TRAPP, an interactive computer program for predicting the density and transport properties of hydrocarbon mixtures by corresponding-states methods has been available for some time and has been well received. A newer formulation, SUPERTRAPP, which covers a more extensive range of fluids and provides data for thermodynamic properties as well, is being validated and documented. When issued, this will replace TRAPP.

Releases were issued recently by IAPS on the viscosity and thermal conductivity of water and steam. These were largely based on work done at the University of Maryland.

A monograph containing critically evaluated correlation equations for the density, surface tension, electrical conductance, and viscosity of molten salts and binary molten salt systems is in preparation. This will provide comprehensive, up-to-date coverage of the field.

Chemical Kinetics

Data in this area are generated by the Chemical Kinetics Data Center and the Ion Kinetics and Energetics Data Center at NBS, the Radiation Chemistry Data Center at Notre Dame, and grant projects at Boston University and the Aerospace Corporation.

The Chemical Kinetic Data Center has completed the task of evaluating a basic data set needed in combustion chemistry. It provides complete coverage of all possible reactions of all possible species involved in the combustion of the C_1 to C_5 alkanes. This work will be published in three volumes, the first of which is already in press.

A comprehensive bibliographic database for combustion is also in preparation and about ready for publication.

A comprehensive paper on triplet-triplet absorption spectra from the Radiation Chemistry Data Center is in press, as is a review of the kinetic data for transients in aqueous solutions containing actinides.

John R. Rumble, Jr., Program Manager

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

Table 1

OSRD Materials Properties Data Program

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

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

Table 2

Major NBS-Outside Data Agreements

Society	Data Area
American Society for Metals	Alloy Phase Diagrams
American Ceramic Society	Phase Diagrams for Ceramists
International Centre for Diffraction Data-JCPDS	Crystal Data
National Association of Corrosion Engineers	Corrosion Data

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

Table 3

OSRD Materials Properties Data Program - FY 86

Structure and Characterization
- Crystallography
  - NBS Crystal Data Center
  - Evaluation Models for Powder Diffraction Data - JCPDS-ICDD
  - Cambridge Crystallographic Data Centre
  - Cation-Nitrogen Distance - University of Illinois - Chicago
- Surfaces
  - ESCA Data Project - Surfax (CA)
  - Ion Sputtering - NBS
  - Low-Energy Electron Diffraction - Oregon State University

Physical Properties
- Molecular Weight of Polymers - NBS
- Properties of Glassy-Forming Melts - Alfred University

Phase Equilibria
- Alloys
  - NBS Alloy Phase Diagram Data Center
  - NBS/ASM Phase Diagram Program
    - Al, Ti - NBS
    - V, Nb - Ames Laboratory, Iowa
    - Cr - University of Wisconsin - Milwaukee
    - Cu - Carnegie-Mellon University
    - Alkalis - Thermfact, Montreal
    - Actinides - Los Alamos National Laboratory
- Ceramics
  - NBS Phase Diagrams for Ceramists Data Center
  - Modeling of Complex Ceramic Phase Equilibria - Penn State University
  - P, AS, and Sb Semiconductors - University of Utah
  - Molten Salts - Rensselaer Polytechnic Institute
  - Selenides and Telurides - Marquette University
- Thermochemistry
  - Thermochemistry of Alloy and Elements - CINDAS, Purdue University

Corrosion
- NBS Corrosion Data Center
- NBS/NACE Corrosion Data Program
  - Stainless Steels in Aqueous Chlorides - Georgia Tech
  - Crevice Corrosion of Stainless Steels - LaQue Center - North Carolina

Mechanical Properties
- Fracture Toughness - University of Florida
- Fatigue - John Deere
- Creep and Stress Rupture - Metal Properties Council
- Ductile Fracture Toughness of Low-Alloy Steels - University of Florida

The Phase Diagrams for Ceramists Data Center has been implementing its agreement with the American Ceramics Society (ACerS) for a joint program on evaluated data. ACerS has begun fund-raising efforts, and the NBS data center has established vigorous programs in database graphics and thermodynamic modeling.

Performance Properties

Corrosion

The National Association of Corrosion Engineers (NACE) and NBS are now beginning projects under a cooperative agreement which will provide the technical community with evaluated corrosion data. The Metallurgy Division (IMSE) and OSRD have established the NBS Corrosion Data Center to act as the technical focal point of this program. Several projects have been started to gather at the data center major collections of industrial corrosion data. In addition, standard computer formats are being prepared.

Mechanical Properties

OSRD has been working closely with outside groups to address a variety of problems related to mechanical properties data. In particular, the National Materials Property Data Network (MPD Network) has developed a major effort to provide computerized access to materials property data. The Office has interacted strongly with this project and has developed a five-pronged effort involving a prototype system of data evaluation, data standardization, database creation, and user workshops.

One highlight was the start of the prototype of a comprehensive materials data system (MIST - see description below), using funding from DOE, DARCOM, NSF, and NBS. The first phase was demonstrated in January 1986, and Phase II is nearing completion.

The evaluation of mechanical properties data until now has been concentrated in areas of high technology such as nuclear power generation and aerospace. This past year, several evaluation projects have continued, and work in fatigue and fracture data has shown promising results.

Another highlight was the establishment of a new ASTM Committee E-49 on Computerization of Material Property Data. Over 75 persons attended the organization meeting, and already several working groups are developing draft standards. OSRD-funded data work has helped in getting this committee off to a quick start.

The MPD Network will involve linking together many databases on a variety of properties created by interested parties. For such a system to be useful, more databases must be created from the now existing published compilations. NMPDN and OSRD are working together to persuade publishers, societies, and other groups to begin building the needed databases more intensely.

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

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

Structure and Characterization

The structure and characterization of solid materials are extremely important. The identification of unknown substances has always been a major use of evaluated data. The NBS Crystal Data Center has developed powerful techniques for rapidly identifying crystalline substances. The NBS Data Center interaction with the International Centre for Diffraction Data-JCPDS (ICDD-JCPDS) continues. This past year the ICDD-JCPDS has had a research associate at the NBS center working on software to be used with the NBS Crystal Data Identification File. That software is now being distributed by the ICDD-JCPDS with the NBS Crystal Data File.

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

Physical Properties

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

Phase Equilibria

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

The Alloy Phase Diagram Center is the focal point of the NBS/American Society for Metals (ASM) joint program to evaluate all alloy phase diagrams. Over the last year, the major thrust was digitizing over 1,000 diagrams for a new publication for binary alloy systems. The Bulletin of Alloy Phase Diagrams published over 50 new diagrams, and work on prototype databases continued. OSRD supports the program in two major ways: direct support of the data center and support of individual evaluation projects (see Table 3).

A key ingredient to success in this type of project is strong user input from the beginning. To this end, NBS, working with several groups, has set up a series of user workshops addressing the needs in several application areas. The workshops outline detailed needs and will help pave the way for industrial acceptance and support of the system. In 1986 two workshops were held. One workshop was for the petrochemical industry and was jointly sponsored by the American Petroleum Institute and the MPD Network. The other was for Aerospace Engineers, and its sponsors included the American Institute of Aeronautics and Astronautics and the MPD Network. Both workshops were well attended and reports will be issued.

Finally, OSRD has worked closely with the Ceramics Division of IMSE to develop a realistic plan to carry out the recommendations of a workshop on a tribology information system held at NBS in 1985. A multi-agency program has been established with DOE, NSF, and the USAF. To begin, a series of 10 projects will be started with the emphasis on building databases of evaluated data in various areas of tribology.

Summary

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

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. Progress has been made in many areas, as summarized below.

Computing Facilities

We continue to provide reliable state-of-the-art computer resources to our data centers. The OSRD Hewlett Packard 1000 computer facility hardware has been enhanced with two additional 404 megabyte disk drives, an additional, more powerful, magnetic tape drive, an upgraded laser printer, and more terminals, modems, and multiplexors. Further, we are working very closely with individuals knowledgeable about the new NBS phone system to ensure our computer facility will have the best possible communication links to/from our users. We have upgraded the operating system twice during this past year (A.85, 4.0) and are now running under the most current one available. The Data Systems Development Group in coordination with the individuals using the HP 1000 in the Center for Chemical Physics 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 are extremely proud of the increase in our library of available software, both from outside sources and developed in-house. This new software is summarized below.

Software purchased or received from users groups:

CDS Runtime Library Options	
KSAM/1000	(keyed sequential access)
KERMIT	(communications, file transfer)
PRINT	(optional printing formats eliminating spooling)
MAIL	(communication to and between users; SRD served as test site for this HP product)
TEXED	(editor powerful in mixing text and tables)
DEBUG	(new improved version)

Software developed in-house:

- o An automated database tape preparation procedure
- o An automated major back-up system including an incremental back-up with frequent protection of modified files only
- o A Getkey-Setkey program for fast access of phone numbers, room numbers, etc. of data center personnel
- o A user log file with messages about down time, new utilities, etc., automatically announced at log on
- o PT, a print program for all available printers, but specifically designed for producing camera-ready copy of scientific documents on the laser printer
- o RDNBS and WRTAP, read and write tape routines, choice of tape drive, and potential for writing 6250 bpi tapes

This office has kept pace with the general proliferation of microcomputers. In addition to the hardware we had available last year, we've purchased IBM AT machines, a printer for the HP 110, memory for the XT, a tablet and mouse, and surge suppressors. Once again, the list of newly available software is impressive and includes:

MICROSOFT C compiler
PASCAL compiler
PROFESSIONAL FORTRAN compiler
KERMIT (communications)
REFLECTIONS (terminal emulation program)
SCIENTIFIC DESK utilities
NORTON utilities
CHEMBASE (Molecular Design demonstration kit)
dBASE III
WORDPERFECT

Of these, the professional FORTRAN, dBASE III, and WordPerfect have become de facto standard software at NBS.

We are presently in the process of purchasing an HP Vectra microcomputer and are also converting our secretarial word-processing equipment to IBM XT and AT machines with HP laserjet printers using WordPerfect.

We keep abreast of developments with the NBS Consolidated Scientific Computing System $(CS)^2$ and have developed application programs running on it, as appropriate. Staff members in the office are proficient in using these facilities, and we eagerly await the promised new operting system (NOS/VE) to see what enhancements it provides in the area of a full ASCII character set and database management packages.

A newly developed long-range computer plan for Standard Reference Data follows this section on computerization.

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 NBS are processed with relative ease.

We have completed upgrading this composition system to Bedford's state-of-the-art Vision Network System. One immediate advantage is the Canon laser printer (CX) which provides considerably better proof copy than the printronix, and we have recently purchased additional type fonts in order to produce camera-ready copy. Other significant advantages include individual stand-alone workstations, each with a 36-megabyte Winchester disk drive, the ability to use IBM PC's as input devices, the acceptance of any ASCII PC diskette input including files from such common word-processing systems as WordStar, MultiMate, and WordPerfect, and the integration of all components via an enhanced ethernet connection.

The processing of many publications is streamlined by using the HP laserjet printer associated with the OSRD Computing Facility to produce camera-ready copy. As mentioned earlier, programs such as PT have been developed to facilitate the processing of tables for output on the laser printer. This is especially useful to users of the OSRD computer or of the comparable machine in CCP.

Numerical Database Activity

Five new databases have been released in the NBS Standard Reference Database Series.

NBS Standard Reference Database 7, EPSTAR, is an interactive FORTRAN program to calculate data related to electron and positron stopping powers for electrons in 285 materials and positrons in 29 materials for energies from 10 keV to 20 GeV. Database 8, XGAM, is an interactive FORTRAN program providing photon cross sections and attenuation for elements Z = 1 to 100 and energies from 1 keV to 100 GeV. The DIPPR Data Compilation of Pure Compound Properties, Database 11, provides the thermodynamic, physical, transport, and environmental property data for 346 compounds of high industrial priority. MIPROPS, Database 12, includes interactive FORTRAN programs to calculate the thermophysical properties of 12 fluids, and the JANAF Thermophysical Tables, Database 13, provide a compilation of critically evaluated thermodynamic properties of approximately 1800 substances over a wide range of temperature.

In addition to the release of these five new databases, an important development this past year has been the release of two of the databases in the series in PC diskette version. STEAM (Database 10) and MIPROPS (Database 12) are currently available in either magnetic tape or PC diskette form. We anticipate increasing efforts in the area of preparation of PC databases and are discussing alternatives concerning the distribution of Standard Reference Data for personal computers.

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

A complete listing of the present NBS Standard Reference Database Series follows:

NBS STANDARD REFERENCE DATABASES

1. NBS/NIH/EPA/MSDC Mass Spectral Database (1986 Version)
2. NBS Chemical Thermodynamics Database (NBS Tech Note 270)
3. *NBS Crystal Data Identification File
4. NBS Thermophysical Properties of Hydrocarbon Mixtures (TRAPP)
7. Electron and Positron Stopping Powers of Materials (EPSTAR)
8. X-ray and Gamma-ray Attenuation Coefficients and Cross Sections (XGAM)
9. Activity and Osmotic Coefficients of Aqueous Electrolyte Solutions (GAMPHI)
10. **Thermophysical Properties of Water (STEAM)
11. DIPPR Data Compilation of Pure Compound Properties
12. **Interactive FORTRAN Programs to Calculate Thermophysical Properties of Fluids MIPROPS 1986
13. JANAF Thermochemical Tables

* Available from the JCPDS-International Centre for Diffraction Data, 1661 Park Lane, Swarthmore, PA 19081. Phone: (215) 328-9400.
** Also available in PC diskette version.

Also, we continue to press for the inclusion of our numeric files on on-line systems such as STN. Presently, the Mass Spectral Database, the Chemical Thermodynamic Database, and the Crystal Data Identification File are resident on CIS, Mass Spec is also available on Questel, and the CISTI system offers the Crystal Data Identification File.

We were pleased to be able to demonstrate many of our databases and associated software at the Tenth International CODATA Conference in Ottawa in July, as well as at both of the national American Chemical Society meetings (New York, NY, and Anaheim, California).

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.

One major commitment concluded this past year was the complete automation of the programs and files of the Crystal Data Center. Using the OSRD Computer Facility, a specialized database management system was developed to perform all of the necessary functions, including data entry, edit checking, data editing, sorting, searching, and reporting. The system is debugged and completely operational.

The other commitment is to the automation of the numeric data files for the Atomic Energy Levels Data Center and the Atomic Transition Probabilities Data Center. The specification and design of a computerized database system of atomic spectroscopic data is complete, including the description of data elements and their relationships and the design of the file structure. Programs being developed for entry and validation of new data, editing of existing data, viewing single records, specifying simple queries, and outputting results in intermediate format on either a terminal or a printer will be available by the end of the year.

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 as well as the yearly indexes of the Journal. Other automated activities associated with the Reference Center are complete such as a tracking system for the review and production processes of publications in progress.

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 Metal Properties Council, with DOE in building a Materials Database System, with AIChE on the DIPPR project, and with such international groups as CODATA and IUPAC. These activities continue to be very fruitful.

The SRD Computing Facility and the machine servicing the data centers in the Center for Chemical Physics provide computer resources for the majority of the in-house data centers and projects, as well as for the office itself in carrying out such support functions as the preparation of manuscripts for publication via computer typesetting and the manipulation and actual production of databases for distribution in magnetic form (e.g., tape, disk). These two machines are by design being kept basically parallel in capabilities, and often specific hardware and software items can be shared. These computers are Hewlett Packard 1000's which in February 1985 were upgraded to the A-series machines. Each has 3 megabytes of memory, and together they have 1.9 gigabytes of mass storage. They service about 40 users, 15-20 simultaneously. It is our intent to maintain the compatibility between these two computers.

Presently these two HP machines are providing stable and well-tested computer resources for our users. They are near state-of-the-art, and considerable effort has been expended to accustom the scientists to the operating environment and to develop tools and systems for auxiliary functions such as back-up, file transfer, preparation of camera-ready copy, etc. Basically, these two machines are doing what the users want.

We feel, therefore, that with minor modifications such as the addition of memory and mass storage, as well as some new software, the combination of resources available will be adequate for the next two years. This is in concurrence with the February 1989 date of amortization for this equipment. Anticipating the acquisition of a new machine in FY 89 and knowing full-well the lead time required in a procurement of this size, the preliminary planning process for a major upgrade needs to be begun now.

Our present thinking in considering the alternatives for our long-range plans is based on realistic and cost-effective technology today. We fully realize that as advances such as CD-ROM and networks of ATs become more accessible and well-developed, we will need to modify and enhance the premises set forth in this paper.

In considering a major change of computer resources, three alternatives were outlined:

1. Using the CS^2 (NBS Central Computer Facility)

2. Providing each individual scientist involved in the SRD program with a personal microcomputer

3. Upgrading our two present minicomputers

Weighing the pros and cons of each of these radically different computer environments requires the preparation of a rudimentary list of the general types of uses made of the present computers. They include the following:

- o automation of data center activities
- o building, maintenance, and networking of databases, both numeric and bibliographic
- o shared access to data by multiple centers
- o preparation of manuscripts and tables for publication
- o preparation of databases and software for distribution to users via on-line networks or in transportable media

Using this list, it becomes evident that the option of upgrading our two present minicomputers is the most desirable alternative. A few sentences about the other alternatives are in order.

The present NBS Central Computer Facility is the Cyber 205 with a Cyber 855 front end. It does not support full ASCII, which makes it virtually impossible to do much of our database development. Plans concerning availability of this capability are uncertain, at best. Furthermore, the systems personnel on our HP computers are more familiar with the scientific requirements of the users and are able to provide individualized assistance and attention. Finally, our users have experienced slow response time when accessing the Cyber interactively, and, indeed, often cannot get a port.

Although we will have as many personal computers available as our users require/request, having those as our sole computer resources is not feasible at this time. Certain databases such as that of the Crystal Data Center are too large to be accommodated by personal computers with today's technology. The need for some databases to have shared access also makes individual computers unattractive, and the frequency with which these databases are updated makes it impractical to maintain them on individual machines. Finally, SRD's tape distribution procedures would not presently be feasible from solely AT's.

These two alternatives, the Cyber mainframe and individual personal computers, will certainly be used for specific applications, whenever appropriate. For the major computer resources for the Standard Reference Data program, however, we believe the recommended course is to replace the present two HP 1000 minicomputers with one upgraded central computer facility to serve OSRD and the data centers. In this upgrade, we will be looking for a better machine with such capabilities as

- o 32 bit word (for precision and accuracy)
- o 8 megabytes of memory (to handle larger, more sophisticated programs)

- o 3-4 gigabytes storage (to handle an increased number of applications and larger databases)
- o 40-50 simultaneous users
- o fourth-generation languages and a choice of the next generation database management packages suitable for the handling of our numerical databases
- o more available software so not as many independently written programs are needed
- o enhanced features in such areas as graphics
- o state-of-the-art capabilities in the preparation of output to be used as camera-ready copy
- o a smooth transition from existing hardware and software conventions

In addition to the Hewlett Packard SPECTRUM machine, we will consider the VAX 8700, the IBM 4300 or 4400 series, the Concurrent 3250, and the comparable Prime or Wang machines.

The above list is cursory. As a first step in the implementation of this long-range plan, we propose to have a detailed outline of general specifications and requirements by mid-FY 87. By that time, we will have personally talked with the data centers and will have jointly assessed what capabilities are needed. By this target date, we will also have canvassed potential vendors to determine possible options, including common and unique features of each, as well as costs. Our plan will be updated and made more specific at that time.

This long-range planning document needs to address one more item--that is, the Bedford Composition System which is jointly maintained by OSRD and IRSD. This was upgraded to the state-of-the-art Meteor System less than six months ago. Our contract with Bedford will ensure that we maintain the most current software. The minor procurement of additional type fonts and characters will allow more complete flexibility in preparation of camera-ready copy off the laser printer. Other increased capabilities in the long term include ability to easily transfer files from available word-processing packages (e.g., WordMarc, WordStar, WordPerfect, etc.) and direct communication links into the system and to the videocomp at GPO.

DATA CENTERS

ATOMIC COLLISION CROSS SECTION DATA CENTER

Jean W. Gallagher, Director
Center for Basic Standards

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 the Center has collaborated with a number of visiting scientists to produce evaluated data publications. Work concentrated on completion of a major review article for Physics Reports entitled "Collisional Alignment and Orientation of Atomic Outer Shells. I. Direct Excitation by Electron and Ion Impact." An evaluated compilation on photoionization and fragmentation of molecules is being completed. Work continues on an in-depth review of measured cross sections for electron-impact optical excitation functions for atoms and atomic ions. The Center is contributing to the preparation of a review entitled "Near-Threshold Electron-Molecule Collisions: Theory and Experiment," and is participating in a critical survey of data on the spectroscopy and kinetics of ozone in the upper atmosphere. In a collaboration with the Controlled Fusion Data Center at Oak Ridge National Laboratory, work continues on the update to "Atomic Data for Controlled Fusion Research."

Approximately 1100 numerical data files have been entered into the Atomic Collisions Data Base. These are being used to prepare figures supporting the Center's review activities. Programs are being developed to provide an online enquiry capability.

Plans for the coming year include beginning two new projects: a second part of the review on collisional alignment and orientation parameters and an evaluated compilation of cross sections for photoionization of atomic ions. The possibility of a collaboration with the Ion Kinetics and Energetics Data Center on an evaluated compilation of ion-molecule reaction rates is being explored.

ATOMIC ENERGY LEVELS DATA CENTER

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

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

Our new energy-level compilations for the 235 spectra of the iron-group elements potassium through nickel (Z=19-28) were published in a one-volume supplement to the J. Phys. Chem. Ref. Data. We completed and published the most extensive compilation of data for (forbidden) magnetic-dipole transitions ever carried out. The data include 1660 predicted wavelengths and transition probabilities (10 nm to 26 mm) for atoms and ions of the elements beryllium through molybdenum. These tables will be used extensively for diagnostics and analysis of radiation from laboratory (tokamak, etc.) and astrophysical plasmas. We have completed critical evaluation and compilation of the energy-level data for more than half of the 42 spectra of molybdenum, an element of special interest for tokamak-discharge diagnostics. A separate compilation giving wavelengths and energy-levels classifications for the spectra of Mo^{5+} through Mo^{41+} is almost ready for submission for publication. We also collaborated with a Japanese group on a similar compilation for spectra of the nickel ions Ni^{8+} through Ni^{27+} (manuscript in preparation).

We are critically reviewing and compiling data on energy levels for the spectra of sulfur and chlorine. The results of new calculations, theoretical interpretations, and measurements stimulated by our reviews are being included in these compilations.

We monitor the literature on atomic energy levels, wavelengths, wavefunctions, etc., and the resulting reference files and published bibliographies are used by a wide clientele. We plan a fourth supplement to our Bibliography on Atomic Energy levels Level and Spectra, covering the period from January 1984 through December 1987. (A. Robey, R. Zalubas)

ATOMIC TRANSITION PROBABILITIES DATA CENTER

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

The Center's purpose is to compile, evaluate, and disseminate data on radiative transition probabilities for atoms and atomic ions. These data are essential in such areas as plasma modeling and analysis, including fusion research, as well as laser physics and astrophysics.

The comprehensive compilation of atomic transition probability data for allowed lines in the elements scandium through nickel is close to completion, but some work remains on evaluating and tabulating data on forbidden transitions in these elements and on transitions in the Be and He isoelectronic sequences. A book "Spectroscopic Data for Iron," assembled from existing NBS-NSRDS data compilations, was published as Volume IV of the ORNL series of books "Atomic Data for Fusion" and was widely distributed among the magnetic fusion community. A second book containing spectroscopic data for Ti and Ni ions is in preparation. A similar special compilation of data for higher ions of Ni, which includes atomic energy level diagrams, is in preparation in collaboration with scientists of the Japan Atomic Energy Research Institute.

Future plans call for completing the compilation of transition probabilities for scandium through nickel, at which point our work will shift to the light elements hydrogen through neon, as well as selected heavy elements (such as Kr and Zr). It is also planned to complete work on both input and output capability for the bibliographic database system. Input of

references on atomic transition probabilities will be initiated. Long-range plans include the design and development of a computerized database of critically evaluated data on atomic spectroscopic quantities.

FUNDAMENTAL CONSTANTS DATA CENTER

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

The Center provides a centralized source of information on the fundamental physical constants and on closely related precision measurements. It participates in the periodic development under the auspices of CODATA of sets of "best" or recommended values of the fundamental physical constants by means of least-squares adjustments. The self-consistent best values of the constants resulting from an adjustment are required for computational purposes and often are the basis for other data compilations. The Center also publishes a quarterly preprint and reprint newsletter entitled "Preprints on Precision Measurement and Fundamental Constants" or PMFC; participates in the organization of conferences relating to the precision measurement-fundamental constants (PMFC) field; administers the NBS Precision Measurement Grant program; and participates in the work of various committees in the PMFC field.

The major activity of the Center during FY 86 involved working towards the completion of the 1986 least-squares adjustment of the constants. The set of best values resulting from this adjustment will replace the now nearly obsolete set resulting from the 1973 adjustment. The 1986 effort, like its 1973 predecessor, is being carried out by B. N. Taylor in collaboration with E. R. Cohen, Rockwell International, and under the sponsorship and guidance of the CODATA Task Group on Fundamental Constants. (Dr. T. J. Quinn, Deputy Director of the International Bureau of Weights and Measures, is current Task Group Chairman.) As part of this effort, a first draft was nearly completed of a document entitled "Recommended Consistent Values of the Fundamental Physical Constants, 1986, Report of the CODATA Task Group on Fundamental Constants, March 1986." Additionally, the Center hosted a meeting of the CODATA Task Group on Fundamental Constants under the guidance of its chairman, just prior to the 1986 Conference on Precision Electromagnetic Measurements held 23-27 June 1986 at NBS Gaithersburg.

The principal focus of the Center during FY 87 will be the completion and publication of the 1986 least-squares adjustment; it is expected that a CODATA Bulletin giving the new set of recommended values will be published in late 1986 and that a more detailed document will be submitted for publication to the Journal of Physical and Chemical Reference Data no later than April 1987.

MOLECULAR SPECTRA DATA CENTER

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

The Center provides for the collection, evaluation, and dissemination of molecular spectral frequencies and other molecular constants. Published reviews are designed to aid in the analysis and identification of compounds

and to permit the determination of a wide range of molecular properties. One phase of the Center's work emphasizes microwave spectra of interstellar molecules.

In January a paper entitled, "Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions - 1985 Revision" was published in J. Phys. Chem. Ref. Data. This review provides the most accurate transition frequencies available for the 59 known interstellar species. It contains about 2545 transitions for 114 isotopic forms of these species. Also included are 1723 transitions whose molecular source is unidentified.

Near the end of the year we plan to complete a review on the microwave spectra of hydrocarbons as part III of the series "Microwave Spectral Tables." This will contain critically evaluated rotational spectra and molecular constants, e.g. rotational constants, dipole moments, for all species with empirical formula C_xH_y.

PHOTON AND CHARGED PARTICLE DATA CENTER

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

The Center compiles, evaluates, and disseminates data on the interaction of ionizing radiation with matter. The data on photons and charged particles include single-scattering cross sections as well as transport data pertaining to the penetration of radiation through bulk matter.

Activities during the past year include the following: (a) Through the synthesis of various theoretical approaches, a method has been developed for the accurate evaluation of the bremsstrahlung spectrum produced in Coulomb interactions between electrons and atoms. Extensive tabulations of these cross sections have been completed for all elements with atomic numbers Z = 1 to 100, for electron energies between 1 keV and 10 GeV. The results have been published in two articles in technical journals, and a computer-readable tape of bremsstrahlung cross sections has also been prepared. (b) A predictive algorithm has been further developed which generates photon scattering, absorption, and pair-production cross sections, as well as attenuation coefficients, for any compounds of specified composition. This algorithm has been incorporated into NBS STANDARD REFERENCE DATABASE 8 (X-ray and Gamma-ray Attenuation Coefficients and Cross Sections) issued by the Office of Standard Reference Data. (c) The energy-loss cross sections for light-charged particles compiled in the Data Center have been used to develop NBS STANDARD REFERENCE DATABASE 7 (Electron and Positron Stopping Powers of Materials) issued by the Office of Standard Reference Data. (d) Preliminary tables have been prepared of proton stopping powers and ranges from about 200 materials in the energy 1 keV to 1 GeV. These tables were generated using Bethe's stopping power theory above, and experimental data below, ~1 MeV.

SPECTROSCOPIC PROPERTIES OF EXCITED ELECTRONIC STATES OF SMALL POLYATOMIC TRANSIENT MOLECULES

Marilyn E. Jacox
Center for Chemical Physics

During the first year of this two-year project, all of the relevant files on the ground-state vibrational energy levels of transient molecules and on the scientific literature pertaining to transient molecule spectroscopy have been transferred to a new, more efficient computer system and have been kept current. The format of the tables of electronic spectral data for polyatomic transient molecules possessing from 3 to 6 atoms has been planned. Data entry is complete for 46 molecules. All of the references have been searched and entered in the final files, together with part of the data, for 105 additional molecules.

The above search has, with a few exceptions, focused on the literature of optical spectroscopy. Before the data are published, the literature on the photoelectron spectroscopy of small molecules will also be surveyed, in order to add further information on the electronic energy levels of small polyatomic molecular ions.

A detailed assessment has been made of typical magnitudes of shift in the electronic band origins and excited-state vibrational spacings associated with valence transitions of small molecules isolated in rare-gas and nitrogen matrices, compared to the gas-phase values. This assessment, which includes diatomic as well as polyatomic molecules, will be summarized in the final electronic energy data compilation, in order to provide guidelines for users who need to estimate the positions of gas-phase band origins for which only matrix isolation data are available.

DATA CENTERS

AQUEOUS ELECTROLYTE DATA CENTER

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

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

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

The thermodynamic properties of calcium chloride solutions have been correlated as functions of temperature and composition. Values for excess Gibbs energies, enthalpies, and heat capacities have been evaluated for concentrations from 0 to 11 molal between temperatures of 298 and 373 K. These results are being published in the CODATA Thermodynamic Tables. Extension to higher temperatures and inclusion of a pressure as an independent variable are underway using an extension of Pitzer's approach.

A project for DIPPR to prepare reference data on the thermodynamic properties of aqueous electrolyte systems as a function of temperature for industrial use is getting underway.

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

CHEMICAL KINETICS DATA CENTER

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

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

A monograph on combustion chemistry entitled "Chemical Kinetic Data Base for Methane Combustion" has been submitted to JPCRD for publication. It contains data on 235 reactions.

Data have now been evaluated for all possible reactions of all possible species involved in the combustion of the C_1 to C_5 alkanes, and methods for extrapolating these data in temperature and pressure have been prepared. The data cover 563 elementary chemical reactions.

Work has started on the extension of the combustion data base through the evaluation of the reactions of atomic and free radical species. The first reactive species to be considered is atomic oxygen. An evaluation of the reactions of atomic oxygen with unsaturated organic compounds has been carried out and will be submitted to JPCRD.

The compilation of chemical kinetic data for combustion chemistry, which consisted of several distinct files set up at different times, has been put into a common format. This compilation is a much larger data base than the comparable evaluated data base, containing data on upwards of 1700 elementary reactions. This is the core data base that will be used for development of a general data base containing data on all gas phase chemical reactions. This task involved the entry of data published between 1977 and 1982, and the reformatting and further annotation of data previously abstracted and published as NBSIR 81-2254 (1981), which covered the literature published between 1971 and 1977.

The center continues to provide support to the NASA stratospheric chemistry program. Robert Hampson was one of the authors of the recently released report to Congress which warned of the consequences of a global warming trend. The role of trace gases in promoting the greenhouse effect means that trace atmospheric-constituent chemistry is of great importance. For that reason we are initiating a new program with NASA support to reconsider the existing data base.

In addition, evaluation activities in the area of halogen chemistry have continued, including participation on the NASA Panel for Data Evaluation.

CHEMICAL THERMODYNAMICS DATA CENTER

Malcolm Chase, Director
Center for Chemical Physics, NBS

The Center provides the chemical process and related industries with critically evaluated thermodynamically consistent data which can be used to establish the equilibrium constants and heats of reaction for important chemical reactions. These critically evaluated data also are used in the design and interpretation of research in physics, chemistry, biochemistry, geochemistry, environmental science, metallurgy, and other fields where chemical interactions are important. The Center provides data describing the change in the chemical properties of substances as well as bibliographic reference services on thermochemistry. In particular, the Center provides enthalpies and Gibbs energies of formation, entropies, C_p in the standard state at 298.15 K and 1 bar, and enthalpies of formation at 0 K for inorganic substances and simple organic substances, and to a more limited extent, transition properties and thermal functions. The publication "The NBS Tables

of Chemical Thermodynamic Properties" (1982) represents a major activity of the Center. It lists 26,000 data values pertinent to 14,000 substances. The experience gained in this work is now being applied in an international cooperative program under the auspices of CODATA.

The Center is cooperating with four others to design an ongoing system for evaluating thermodynamic data. Together they have produced a set of prototype tables. These tables, covering a number of compounds of calcium and some auxiliary substances, serve two purposes. One, they demonstrate the feasibility of producing chemical thermodynamic tables using decentralized highly-automated cooperative activities of a number of data centers in accordance with the system outlined in CODATA Bulletin No. 47, "A Systematic Approach to the Preparation of Thermodynamic Tables." Two, they provide a model for a new generation of tables. These tables will be published by CODATA and made available for review and comment by the thermochemical community.

In another CODATA-related activity, the monograph on the CODATA Key Values has been prepared for publication. A paper on the reaction catalog for rubidium compounds is also in press.

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

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

The JANAF Thermochemical Tables will now be prepared as part of the activities of the data center. These cover the thermodynamic properties for the crystal, liquid, and ideal gas state over a wide temperature range. Properties covered are heat capacity, entropy, Gibbs energy function, enthalpy, enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant for formation of each compound from the elements in their standard reference states.

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

A revised and updated comprehensive edition of the JANAF Tables is in press as a Supplement to the Journal of Physical and Chemical Reference Data.

FLUID MIXTURES DATA CENTER

Neil A. Olien, Chief
Thermophysics Division
Center for Chemical Engineering, NBS

The Center is organized to compile and evaluate data on the thermodynamic and transport properties of fluids and fluid mixtures. These properties include formulations for the density and other thermodynamic properties of pure fluids, the viscosity and thermal conductivity of pure fluids, and the same properties for fluid mixtures. The Center is also involved with the development of techniques to predict transport properties of pure fluids from thermodynamic and molecular data, to predict properties of mixtures from the properties of pure fluids, and to interpolate and extrapolate data for properties over 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 data bases which are then disseminated by OSRD and other organizations.

A computer package called MIPROPS has been completed and documented which includes all of the fluids of "Thermophysical Properties of Fluids - I" and "Thermophysical Properties of Fluids - II." The package therefore calculates properties for hydrogen, helium, nitrogen, oxygen, argon, ethylene, nitrogen trifluoride, methane, ethane, propane, isobutane, and normal butane. The package will be available from OSRD in the fall of 1986 in standard tape version and on microcomputer disk, which is designed to be compatible with most personal computers.

A paper giving evaluated data for carbon monoxide equilibrium properties is complete and published, a paper on methanol is nearing completion, and a paper on the transport properties of argon is in JPCRD review.

The predictive computer code SUPERTRAPP is in the final testing stage. When test and validation have been completed, it will be made available on magnetic tape through OSRD. It will replace the current version of the TRAPP computer package. This should take place in late 1986 or early 1987.

Future plans include theoretical studies leading to the development of new mixing rules, completion of a computer package called DDMIX, critical evaluations of the properties of benzene and toluene, and completion of the corresponding-states studies for the methane-ethane system.

ION KINETICS AND ENERGETICS DATA CENTER

Sharon G. Lias, Director
Center for Chemical Physics

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.

In the past year the Data Center has concentrated on completing a major publication, a compilation of evaluated heats of formation of more than 5,000 positive and negative ions which will include evaluated ionization energy and

electron affinity data. Work during the year on this project included addition of all the data which had appeared in the literature during the years 1981-1986 (i.e. data on approximately 1400 species). A review of the field, to be included as introductory textual material, has been written, and ink drawings of the recently-added compounds are now being prepared. The publication will be submitted to the Journal of Physical and Chemical Reference Data on or before January 1, 1987.

The data base for the 1984 Data Center publication of 780 evaluated gas basicities/proton affinities of neutral molecules was brought up to date during the past year by the addition of all the data which appeared in the literature since the cut-off date of the original publication (1984). New data for 234 species were added, and some of the values of proton affinities were re-evaluated as a result of the appearance of better experimental or theoretical data.

Plans for the coming year include initiation of a project on the evaluation of rate constants for ion/molecule reactions in collaboration with the Atomic Collision Cross Section Data Center (CBS), the Jet Propulsion Laboratory, and the Air Force Geophysical Laboratory.

MOLTEN SALTS DATA CENTER

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

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

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

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

NATIONAL CENTER FOR THE THERMODYNAMIC DATA OF MINERALS

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

The Center compiles, indexes, and evaluates data on the thermodynamic and thermophysical properties of minerals, their synthetic analogs, and geologic materials. These data are important for geochemical purposes and useful industrially in the fields of metallurgy and the synthesis and production of inorganic chemicals.

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

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

RADIATION CHEMISTRY DATA CENTER

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

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

Support of the Center is shared by OSRD and the DOE Office of Basic Energy Sciences.

A critical review on triplet-triplet absorption spectra data is in press, and a review on kinetic data for transients in aqueous solution has been submitted for publication. Other data compilations in progress include: intersystem-crossing quantum yields, one-electron reduction potentials involving radicals in aqueous solution, and rate constants for transients from water.

Several programs for automation of the Center are underway. These include programs to produce and prepare for publication tables of data indexes and reference lists. Programs for on-line searching of numerical data files are also being developed.

Publication of the biweekly and cumulative bibliographies is being continued.

THERMODYNAMIC RESEARCH CENTER

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

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

The Center has continued its work on the thermodynamic properties of organic substances containing the atoms C, H, and O in the C_1 - C_4 range. A substantial number of major industrial products and intermediates is included in this group. Entropies and enthalpies for the condensed phases of all substances in the group for which low-temperature heat-capacity data are available have been gathered and evaluated. A paper has been published in JPCRD. In another part of the same project, ideal-gas thermal functions have been prepared for those molecules in the group for which sufficient data are available. A paper is in press. A third portion of the work involves the thermochemistry of these substances. Available enthalpies of reaction (primarily enthalpies of combustion) and equilibrium constants have been evaluated. These are being combined to provide formation properties and ideal-gas and condensed-phase thermal functions for as many substances as possible.

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

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.

A primary objective is the development of techniques for the evaluation of data for solutions over a range of temperatures and for solutions containing two or more electrolytes. An extension of Pitzer's method for mixtures has been developed as has a 3-dimensional spline fit for high-temperature systems where pressure must be taken into account along with temperature and concentration. Data on $CaCl_2$ solutions up to 325°C are being evaluated.

OSRD Database 9, GAMPHI, which gives the activity coefficients of aqueous electrolyte solutions at room temperature has been rewritten to run on a microcomputer and has been extended to work for solutions containing two or more electrolytes.

CHEMICAL THERMODYNAMIC PROPERTIES OF POLYCYCLIC AROMATIC HYDROCARBONS

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

Tables of standard chemical-thermodynamic properties of polycyclic aromatic hydrocarbons are being calculated from the best available data and extended to higher temperatures and higher carbon numbers by use of the Benson method. These tables for the ideal gas phase are to cover 298 K to 3000 K because of the importance of these data in understanding soot formation in flames and the high-temperature vaporization of graphite. As the number of 6-member rings increases, the number of different structures with the same number of carbon atoms increases and the number of isomers increases. Where isomerization occurs isomer-group thermodynamic properties and distributions within isomer groups are to be calculated. At fixed hydrogen partial pressures, polycyclic aromatic hydrocarbons with the same numbers of carbon atoms become isomers, and therefore it is of interest to calculate chemical thermodynamic properties for these enlarged 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 comprehensive formulations for the thermodynamic and transport properties of fluids. This includes formulations providing an accurate description of behavior in the critical region.

A revised and extended scaled equation of state consistent with the predictions of the renormalization-group theory has been developed and applied for the preparation of reference data in the critical region for several fluids. A new technique which permits an automatic transformation from a scaled formulation to a classical formulation without an ad hoc crossover function is being developed.

Representative equations for the transport properties of fluids that include a characterization of the singular behavior of these properties near the critical point consistent with the mode-coupling theory of critical dynamics have been developed. These were applied to the preparation of releases on the viscosity and thermal conductivity of water and heavy water for the International Association for the Properties of Steam.

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

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

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

The techniques are being applied to the eleven gases; N_2, O_2, CO, NO, CH_4, CF_4, SF_6, CO_2, N_2O, C_2H_4, C_2H_6, to the 55 mixtures they form among themselves and the 44 mixtures these gases form individually with the noble-gas set Ne, Ar, Kr, Xe. Correlations are being carried out for the viscosity, second virial coefficient, isotopic and binary diffusion coefficient, thermal diffusion factor, and thermal conductivity from 100-3000 K at atmospheric pressure.

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

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

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

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

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

Formulations for the thermodynamic properties of the individual fluids and for air have been prepared using a common formulating technique. Although the formulations for the individual fluids can be used to provide a formulation for air considered as a mixture of the three in the gas phase, this technique is less successful in calculating phase equilibria. The mixture properties in the critical region are also a problem. Corresponding states and other techniques are being evaluated as methods to solve these problems and to develop an accurate wide-ranging formulation for air.

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

This project is intended 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 will also be estimated where possible. The method will use 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 ΔG_f's ($\pm$ 0.4 kJ) can be obtained for many of these compounds. All the available equilibrium constants and third law ΔG_f's will be examined and used to obtain a reliable set of ΔG_f, ΔH_f and S° 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 ΔG_f's for a large number of organic compounds useful to biochemists, organic chemists, and industrial chemists.

The work is being carried out cooperatively with the Aqueous Electrolyte Data Center.

DIPPR DATA PROJECTS

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

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

Currently, NBS is involved directly with two DIPPR activities. One is the preparation of automated products for the DIPPR Data Prediction Manual. This manual contains a variety of methods for predicting or estimating various types of data needed in the chemical process industry. These automat-ed methods currently involve computer algorithms suitable for making the necessary calculations, but the ultimate goal is preparation of an interactive computer program for prospective users.

The other activity is a project to prepare evaluated data on the thermodynamic properties of aqueous solutions over a range of temperatures. This work is being carried out at the Aqueous Electrolyte Data Center.

A handbook on aqueous electrolyte solutions for engineers has recently been published. This handbook provides data, estimation techniques, references, and theoretical background for a range of technical problems an engineer might be expected to face. It is similar to the Data Prediction Manual but is focused on aqueous electrolyte systems.

PROPERTIES OF POLAR FLUIDS

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

A model for the thermodynamic surface of polar mixtures is being developed as an expansion about a physical model. An important advantage of this approach is that values for the molecular parameters for the model afford a means of establishing the thermodynamic consistency between the various sets of measurements. (A major limitation to accuracy for any correlation of thermodynamic data are inconsistent data, even for pure fluids). The expansion terms are so constructed that the formulation reduces to the very accurate existing surfaces for the pure components at the concentration limits.

The model is being applied to the mixture of H_2O and CO_2.

Results to date include fits to the pure components and the derivation of the appropriate molecular parameters for these. Fits on isotherms now are being made to PVT measurements to obtain values for cross-interaction molecular parameters for each set of mixture measurements. In the analysis, special attention is paid to the second virial coefficient for the cross interaction. Fortunately, very accurate measurements exist for values of excess enthalpy for dilute mixtures. Thus not only is it possible to intercompare sets of PVT measurements, but also compare them with enthalpy measurements, a different kind of measurement.

The task of selecting a data base for the global fits should be completed by the end of this fiscal year. A number of the terms in the expansion have been determined by the condition that the formulation reduce to the existing formulations for the pure component at the concentration limits.

CRITICAL EVALUATION OF HIGH-TEMPERATURE KINETIC DATA

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

This project compiles and disseminates evaluated data sheets describing the high-temperature kinetics of selected chemical reactions found to occur in rockets and jets. The data sheet format is now firmly established. A total of 79 data sheets have been compiled to date. Major categories covered are: the H_2-O_2 system, hydrocarbon oxygen systems, hydrogen-halogen systems, metal-oxygen systems, O_2 energy-transfer processes, haloalkene-O_2 systems, and NH_3-O_2 systems.

PROPERTIES OF TRANSITION METAL COORDINATION COMPLEXES

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

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

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

BINARY VAPOR-LIQUID EQUILIBRIUM DATA FOR LIGHT HYDROCARBONS WITH METHANE

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

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

DATA CENTERS

ALLOY PHASE DIAGRAM DATA CENTER

J. B. Clark, Director
Institute for Materials Science and Engineering, NBS

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

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

A vigorous evaluation program for titanium systems, with support by ONR, has been completed, and a monograph on titanium binary systems is in final stages of preparation. It will be issued as an ASM monograph. Evaluation of aluminum systems has continued, supported in part by DARPA. During this evaluation effort, thermodynamic optimization programs have been enhanced and interfaced with the graphics software.

The prototype user-friendly phase diagram database of graphical and numerical information is now complete. A new effort was completed to provide 1500 digitized binary phase diagrams for the new ASM compendium, Binary Alloy Phase Diagrams.

CORROSION DATA CENTER

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

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

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

The first database of corrosion data has been completed and will be released for personal computers. This contains kinetic and thermodynamic data from traditional data sources and will provide the basis for future database activities.

CRYSTAL DATA CENTER

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

The Crystal Data Center is concerned with the collection, evaluation, and dissemination of data on solid-state materials. The Center maintains a database which includes chemical and crystallographic information on all types of substances with known unit cells. The materials fall into the following categories: inorganics, organics, organometallics, metals, intermetallics, and minerals. For each substance, there are a variety of input and derived data parameters including: the conventional and reduced cell parameters, the space group, the compound name and formula, calculated density, literature reference, and critical comments. During the past year, the database has been significantly upgraded and expanded.

To permit scientists to use the database, we have developed software tools that can be distributed with the database or used to search the database on-line at a central site. NBS software (NBS*LATTICE), which is an integral part of the CRYSTAL DATA Distribution Package, is designed to be used on a variety of computers. With the lattice-matching program function, unknown compounds can be identified by comparison with entries in the database once any cell of the lattice has been determined using diffraction techniques. The lattice-matching method offers an excellent technique to characterize solid-state materials and is now in routine use at the National Bureau of Standards, in industrial analytical laboratories, and crystallographic data centers.

Using the on-line CISTI-NBS CRYSTAL DATA Search System, the database can be accessed by scientists worldwide. All key data items can be searched and answers to queries can be obtained by using highly efficient Boolean-type searches. During the year, this system has been used by the NBS Crystal Data Center and by individual scientists to solve a variety of scientific problems in diverse areas of chemistry and solid-state physics.

Future efforts of the Crystal Data Center will focus on several areas of activity. First, in 1987 the next version of the NBS CRYSTAL DATA Distribution Package will be released. Both the database and the software components of this package will be upgraded. The database will be expanded seven times over the present version and will include 115,000 entries with 1.7 million data records. Second, minerals data will be processed and evaluated in order to produce a comprehensive minerals subfile with at least one entry for each known mineral. Third, research will be carried out, scientific software will be developed, and scientific papers on CRYSTAL DATA products will be written.

PHASE DIAGRAMS FOR CERAMISTS DATA CENTER

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

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

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

During the current year, significant progress has been made in the computerization of the database. More than 5,000 bibliographic entries have been keyboarded. A software package for efficient digitization, editing, and plotting of binary ceramic phase diagrams is now being used routinely. Binary phase diagrams were plotted in camera-ready form using this system, and work has progressed on a similar package for ternary systems, specifically designed for the most efficient use in this data center. Volume 6 of the PDFC Series will be completed in late 1986.

During the next year, the momentum of the database computerization effort will continue to increase. Funds from the ACerS fund-raising activity have become available to support ACerS research associates to work at NBS and assist with the task of database development. The utilization of thermochemical optimization and computer modeling methods in evaluation will be increased.

PROJECTS

ANALYSIS OF TIME-DEPENDENT ELEVATED TEMPERATURE DATA

M. Prager
The Metal 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 for 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 and Niobium Alloys

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

Titanium Alloys

J. Murray
National Bureau of Standards
Gaithersburg, Maryland
Source of Support: ONR

Alkali Metals

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

Chromium Alloys

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

Actinide Alloys

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

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

CATION-NITROGEN DISTANCE IN NITRIDES OF CRYSTALLINE COMPOUNDS

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

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

COMPUTER EVALUATION MODELS FOR POWDER DIFFRACTION DATA

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

Powder diffraction analysis is perhaps the technique most widely used to identify solid materials. In recent years, new computer methods for evaluating these data have been developed and applied to the powder data collection, identifying many problems. This project has examined all problem powder data to resolve the problems.

CORROSION RATE DATA FOR STAINLESS STEEL

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

This is a pilot project in the NBS/NACE corrosion data program. The objective is to compile and evaluate corrosion rate data for austenitic stainless steels in aqueous chloride solution and to organize the data in suitable formats for presentation and retrieval. An important part of this effort has been to identify the parameters which are important for the evaluation of corrosion susceptibility of these steels.

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: NBS

The Cambridge Crystallographic Data Centre has had a continuing collaboration with the NBS Crystal Data Center. The Cambridge Centre supplies numerical crystallographic data and references for organic and organometallic materials. From these entries, selected information will be used to update the NBS Crystal Data ID File, which is available for on-line use.

DUCTILE FRACTURE TOUGHNESS OF HIGH-STRENGTH LOW-ALLOY STEELS

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

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

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

ESCA DATA BASE PROJECT

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

Electron Spectroscopy for Chemical Analysis (ESCA) is a technique that has proved of wide importance in characterizing the surface composition of materials. The present project is concerned with creating a database of critically evaluated line energy data for ESCA. One interesting aspect of this project is the use of a personal computer in building the database. Over 10,000 data records have been evaluated.

EVALUATION OF INORGANIC CRYSTALLOGRAPHIC DATA

J. Messick
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 NBS and the JCPDS. The data come from both the University of Bonn and the JCPDS Powder Diffraction File.

FATIGUE PROPERTY DATABASE

S. Foss
John Deere Technical Center
Moline, Illinois
Source of Support: DOE

The analysis of mechanical property data has become very important as the materials community improves the quality of property data for alloys. This project is incorporating several fatigue analysis techniques into a personal computer database so that future analysis can be carried out efficiently.

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

J. McCarthy
Lawrence Berkeley Laboratory
Berkeley, California

J. Westbrook
W. Grattidge
Sci-Tech Knowledge Systems
Scotia, New York

H. H. Li
CINDAS
Purdue University
West Lafayette, Indiana

B. Parker
Stanford University
Palo Alto, California

H. Mindlin
Battelle Columbus Research Laboratory
Columbus, Ohio

A. Marcus
Aaron Marcus Associates
Berkeley, California

Sources of Support: NBS, DOE, DOD, NSF, NASA, National Laboratories

The MIST demonstration project is a joint effort between NBS and DOE to build a prototype materials data system. During the past two years, two phases have been completed including development of a flexible, extensible database schema and its implementation on the Spires DBMS at Stanford University.

The major goals of the project are twofold:

1. To demonstrate that a comprehensive materials data system can be built

2. To provide a solid foundation for building operational systems in the future.

The initial set of users will be in DOE National Laboratories. Work is being done in close cooperation with the National Materials Property Data Network.

PHASE DIAGRAMS FOR CERAMISTS - OSRD Projects

P, As, and Sb Semiconductors

G. B. Stringfellow
University of Utah
Salt Lake City, Utah
Source of Support: NSF

Molten Salts

G. J. Janz
Rensselaer Polytechnic Institute
Troy, New York
Source of Support: NSF

Selenides and Telurides

R. F. Brebrick
Marquette University
Milwaukee, Wisconsin
Source of Support: NSF

These evaluation projects are an important part of the American Ceramics Society-National Bureau of Standards joint program on evaluating ceramic phase diagrams. The resulting work will be published in the forthcoming volumes of the Phase Diagrams for Ceramists Series.

POLYMER SOLUTION MOLECULAR WEIGHT AND VISCOSITY PROJECT

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

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

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

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 will critically examine all LEED and assess their quality. It will cover elemental surfaces and the compound ionics and semiconductors. Structures formed by adsorption will also be included.

THERMOCHEMICAL MODELING OF COMPLEX CERAMIC PHASE EQUILIBRIA

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

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

THERMODYNAMIC REFERENCE DATA OF ELEMENTS AND BINARY ALLOYS

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

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

Journal of Physical and Chemical Reference Data, Volume 15

No. 1

Triplet-Triplet Absorption Spectra of Organic Molecules in Condensed Phases
Ian Carmichael and Gordon L. Hug

Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions - 1985 Revision
F. J. Lovas

New International Formulations for the Thermodynamic Properties of Light and Heavy Water
J. Kestin and J. V. Sengers

Forbidden Lines in ns^2np^k Ground Configurations and nsnp Excited Configurations of Beryllium through Molybdenum Atoms and Ions
Victor Kaufman and Jack Sugar

No. 2

Thermodynamic Properties of Twenty-One Monocyclic Hydrocarbons
O. V. Dorofeeva, L. V. Gurvich, and V. S. Jorish

Evaluated Kinetic Data for High-Temperature Reactions, Volume 5. Part 1. Homogeneous Gas Phase Reactions of the Hydroxyl Radical with Alkanes
D. L. Baulch, M. Bowers, D. G. Malcolm, and R. T. Tuckerman

Thermodynamic Properties of Ethylene from the Freezing Line to 450 K at Pressures to 260 MPa
Majid Jahangiri, Richard T. Jacobsen, and Richard B. Stewart

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

A Critical Review of Aqueous Solubilities, Vapor Pressures, Henry's Law Constants, and Octanol-Water Partition Coefficients of the Polychlorinated Biphenyls
Wan Ying Shiu and Donald Mackay

No. 3

Computer Methods Applied to the Assessment of Thermochemical Data. Part I. The Estblishment of a Computerized Thermochemical Data Base Illustrated by Data for $TiCl_4(g)$, $TiCl_4(l)$, $TiCl_3(cr)$, and $TiCl_2(cr)$
S. P. Kirby, E. M. Marshall, and J. B. Pedley

Thermodynamic Properties of Iron and Silicon
P. D. Desai

Cross Sections for Collisions of Electrons and Photons with Nitrogen Moelcules
Y. Itikawa, M. Hayashi, A. Ichimura, K. Onda, K. Sakimoto, K. Takayanagi, M. Nakamura, H. Nishimura, and T. Takayanagi

Thermochemical Data on Gas-Phase Ion-Molecule Association and Clustering Reactions
R. G. Keesee and A. W. Castleman, Jr.

Standard Reference Data for the Thermal Conductivity of Liquids
C. A. Nieto de Castro, S. F. Y. Li, A. Nagashima, R. D. Trengove and W. A. Wakeham

Chemical Kinetic Data Base for Combustion Chemistry. Part 1. Methane and Related Compounds
W. Tsang and R. F. Hampson

No. 4

Improved International Formulations for the Viscosity and Thermal Conductivity of Water Substance
J. V. Sengers and J. T. R. Watson

The Viscosity and Thermal Conductivity of Normal Hydrogen in the Limit of Zero Density
M. J. Assael, S. Mixafendi, and W. A. Wakeham

The Viscosity and Thermal Conductivity Coefficients of Gaseous and Liquid Argon
B. A. Younglove and H. J. M. Hanley

Standard Chemical Thermodynamic Properties of Alkyne Isomer Groups
Robert A. Alberty and Ellen Burmenko

Recent Progress in Deuterium Triple-Point Measurements
L. A. Schwalbe

Rate Constants for Reactions of Radiation-Produced-Transients in Aqueous Solutions of Actinides
S. Gordon, J. C. Sullivan, and Alberta B. Ross

Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C_1 to C_4. Part 2. Ideal Gas Properties

Supplements

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

Other Publications in NBS Series

Interactive FORTRAN Program for Micro Computers to Calculate the Thermophysical Properties of Twelve Fluids (MIPROPS)
Robert D. McCarty
NBS Technical Note 1097

Materials Information for Science and Technology (MIST) - Project Overview, Phases I and II and General Considerations
Walter Grattidge, John McCarthy, Clyde Northrup, Jr., and John Rumble,
NBS SP 726

Scientific and Technical Factual Databases for Energy Research and Development Characteristics and Status for Physics, Chemistry and Materials
John Rumble, Joan Sauerwein, and Sharon Pennell

Data Publications from Other Publishers

Bulletin of Alloy Phase Diagrams, Vol. 7, 1986
Joanne L. Murray, Editor
American Society for Metals
(Evaluations done by NBS Alloy Phase Diagram Data Center and OSRD-funded projects)

Ag-Cs	As-Eu	Cu-Na
Ag-k	As-RE	Cu-Rb
Ag-Li	Au-Cs	Cu-Th
Ag-Na	Au-Li	Fe-Nb
Ag-Rb	Au-Na	Fe-Ta
Al-Pt	Au-Rb	Mg-Ti
As-Ce	Be-Cr	S-Ti
As-Dy	Cu-K	Se-Ti
As-Er	Cu-Li	Te-Ti

Bibliographies and Indexes from Other Publishers

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

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

PUBLICATIONS SCHEDULED FOR 1987

Journal of Physical and Chemical Reference Data

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

High Temperature Vaporization Behavior of Oxides
R. H. Lamoreaux and D. L. Hildenbrand

Electrical Resistivity of Niobium and Titanium
R. N. Bogaard, H. M. James, and C. Y. Ho

Thermodynamic Properties of Manganese and Molybdenum
P. D. Desai

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

Compilation and Critical Evaluation of the Phase Diagrams and Thermodynamic Properties of the 70 Binary Alkali Halide System Having Common Ions
James Sangster and Arthur Pelton

The Thermodynamic Measurements of Rubidium Compounds: A Comparison of Measured Values with those Predicted from the NBS Tables of Chemical Thermodynamic Properties
V. B. Parker, W. H. Evans, and R. L. Nuttall

Thermochemical Data on the Gas Phase Compounds of Sulfur, Fluorine and Oxygen Related to Pyrolysis and Oxidation of Sulfur Hexafluoride
John T. Herron

Evaluation of Binary Excess Volume Data for the Methanol & Hydrocarbon Systems
R. Srivastava and B. D. Smith

Evaluation of Binary Excess Enthalpy Data for the Methanol & Hydrocarbon Systems
R. Srivastava and B. D. Smith

The Thermochemistry of Inorganic Solids IV. Enthalpies of Formation of Compounds of the Formula MX_aY_b
W. M. Mohamed and Sidney W. Benson

CODATA Thermodynamic Tables. Selections for Some Compounds of Calcium and Related Mixtures. (A Prototype Set of Tables)
D. Garvin, V. Parker, H. J. White

Standard Thermodynamic Functions of Gaseous Polyatomic Ions at 100 to 1000K
A. Loewenschuss and Y. Marcus

The Viscosity of Carbon Dioxide, Methane, and Sulphur Hexafluoride in the Limit of Zero Density
R. D. Trengove, and W. A. Wakeham

Spectral Data for Highly Ionized Molybdenum, Mo VI - Mo XLII
Toshizo Shirai, Keishi Ishii, Jack Sugar, Kazuo Mori, Yohta Naka, and Kunio Ozawa

^{13}C Chemical Shieldings in Solids
T. M. Duncan

Extinction Coefficients of Triplet-Triplet Absorption Spectra of Organic Molecules in Condensed Phases: A Least Squares Analysis
Ian Carmichael, W. P. Helman, and G. L. Hug

The Mark-Houwink-Sakurada Relation for Poly (Methyl Methacrylate)
Herman L. Wagner

Standard Chemical Thermodynamic Properties of Alkanethiol Isomer Groups
Robert A. Alberty, Ellen Burmenko, Tae H. Kang, and Michael B. Chung

Evaluation of Data Availablility and Quality for Interaction Second Virial Coefficients of Use to the Gas Industry
B. J. Van Wie, M. Langenberg, W. Chang, K. H. Kumar, and K. E. Starling

The Viscosity of Normal Deuterium in the Limit of Zero Density
M. J. Assael, S. Mixafendi, and W. A. Wakeham

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

Evaluated Chemical Kinetic Data for the Reactions of Atomic Oxygen O(3p) with Unsaturated Hydrocarbons
R. J. Cvetanovic

Supplements Scheduled for 1987

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

NSRDS-NBS Series Publication Scheduled for 1987

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

Data Publications from Other Publishers Scheduled in 1987

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

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

Bibliographies and Indexes from Other Publishers Scheduled in 1987

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Vol. 20, 1987
Radiation Chemistry Data Center

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Vol. 19, 1986
Radiation Chemistry Data Center

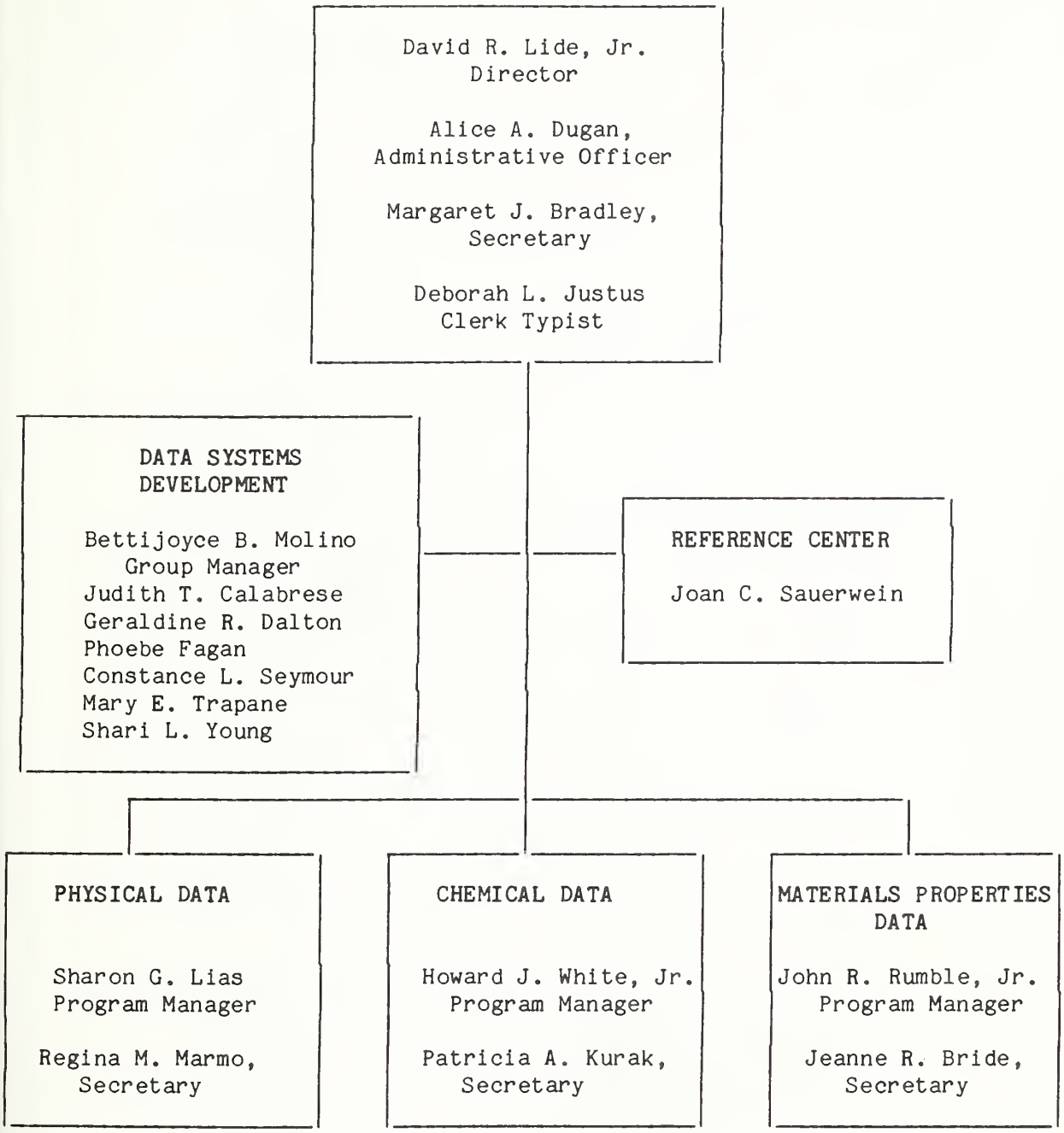
Bulletin of Chemical Thermodynamics, Vol. 27, 1984
Robert D. Freeman, Editor
IUPAC Commission on Thermodynamics and Thermochemistry

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
ASME	American Society of Mechanical Engineers
ASTM	American Society for Testing and Materials
BAPD	Bulletin of Alloy Phase Diagrams
CAC	Center for Analytical Chemistry, NML, NBS
CAD	Computer-Aided Design
CAM	Computer-Aided Manufacturing
CAS	Chemical Abstracts Service
CBS	Center for Basic Standards, NML, NBS
CCE	Center for Chemical Engineering, NEL, NBS
CCP	Center for Chemical Physics, NML, NBS
CINDAS	Center for Information and Numerical Data Analysis and Synthesis, Purdue University
CIS	Chemical Information System
CISTI	Canada Institute for Scientific and Technical Information
CODATA	Committee on Data for Science and Technology (ICSU)
CRR	Center for Radiation Research, NML, NBS
CSIN	Chemical Substances Information Network
DARCOM	Department of The Army Command
DARPA	Defense Advanced Research Projects Agency
DECHEMA	Deutsche Gesellschaft 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, NBS-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
NBS	National Bureau of Standards
NCI	National Cancer Institute
NEL	National Engineering Laboratory, NBS
NIH	National Institutes of Health
NLM	National Library of Medicine
NML	National Measurement Laboratory, NBS
NMPDN	National Materials Property Data Network
NMR	Nuclear Magnetic Resonance
NRC	National Research Council
NSF	National Science Foundation
NSRDS	National Standard Reference Data System
OA	Other Agency (Funding)
OMS	Office of Measurement Services, NML, NBS
ONR	Office of Naval Research
OSRD	Office of Standard Reference Data, NML, NBS
OSTP	Office of Science and Technology Policy
PDFC	Phase Diagrams for Ceramists Data Center
PL	Public law
PMFC	Precision Measurements - Fundamental Constants
PMS	Physical Measurement Services
RCDC	Radiation Chemistry Data Center
SAE	Society of Automotive Engineers
SPE	Society of Plastics Engineers
SRD	Standard Reference Data
SRM	Standard Reference Material
STRS	Scientific and Technical Research and Services (appropriated NBS funds)
TRAPP	Thermophysical Properties of Hydrocarbon Mixtures Database
UNESCO	United Nations Educational, Scientific, and Cultural Organization
USGS	United States Geological Survey

OFFICE OF STANDARD REFERENCE DATA



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

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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.

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Computer typesetting of NSRDS publications via the Bedford Composition System; software control of the Bedford System and user interface to that system

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System manager for OSRD computer facility; user interface and consultant for OSRD computer resources; programming for data automation and dissemiantion.

Mr. Zhou Jiaju
Guest Scientist from Beijing, China

Design and implementation of data center automation; computerized dissemination of Standard Reference Data.

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Processing of files received from outside data centers on Bedford Composition System; user interface to that system; reproduction and inventory control of NBS Standard Reference Database Series.

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

Data input and verification; editing of data files; processing of files on Bedford Composition System.

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

General programming support; support for OSRD computer facility.

PUBLICATIONS BY OSRD STAFF

On the Mechanism of the Reactions of Alkyl Ions with Alkylamines: Competing Proton Transfer and Condensation Reactions", P. Ausloos and Sharon G. Lias, J. Am. Chem. Soc. 108, 1792 (1986).

Absolute Values of Gas Phase Proton Affinities and Basicities of Molecules: A Comparison between Theory and Experiment, D. A. Dixon and Sharon G. Lias, Molecular Structure and Energetics, (1986).

On the Mechanism of Formation of Dialkylhalonium Ions in Alkyl Halides, Z. Karpas and Sharon Lias, J. Org. Mass Spectrom., submitted (1986).

Halomethylenes: Effects of Halogen Substitution on Absolute Heats of Formation, Sharon G. Lias, Z. Karpas, and J. F. Liebman, J. Am. Chem. Soc., 107, 6089 (1985).

Takehiko Shimanouchi and the Codification of Spectroscopic Information, David R. Lide, Journal of Molecular Structure, (1986)

Scientific and Technical Factual Databases for Energy Research and Development - Characteristics and Status for Physics, Chemistry, and Materials, John Rumble, Joan Sauerwein, and Sharon Pennell, (U.S. Department of Commerce, Washington, DC, 1986)

Materials Data: Requirements for the Future, C. J. M. Northrup, Jr. and J. Rumble, Jr., Communications on the MSE Study (Materials Research Society, 1986)

Materials Information for Science & Technology (MIST) - Project Overview, Phases I and II and General Considerations, Walter Grattidge, John McCarthy, Clyde Northrup, Jr., and John Rumble, Jr., SP 726 (1986)

Near Future and Long-Range Goals Necessary for Meeting National Needs for Materials Property Data, John R. Rumble, Jr., 31st International Symposium of SAMPE (Society of Autorated Manufacturing and Processing Engineers, Los Angeles, CA, 1986)

Computerized Materials Property Data Systems, John Rumble, Jr. and J. Gilbert Kaufman, Proceedings, Oceans '86 Conference (IEEE, New York, NY, 1986)

Standard Reference Data Publications 1964-1984, Joan C. Sauerwein and Geraldine R. Dalton (1985)

Properties of Steam, Howard J. White, Jr., Mechanical Engineering, (August 1986)

Steam Tables, Howard J. White, Jr., The Encyclopedia of Physical Science and Technology, (1986)

INVITED TALKS AND PRESENTATIONS BY OSRD STAFF

Structures and Reactivities of $C_6H_5^+$ Ions, Seventh East Coast Symposium on Ion/Molecule Chemistry, University of Delaware, Newark, Delaware, October 1985
Sharon G. Lias

Competing Proton Transfer and Condensation Reactions, 191st National Meeting, American Chemical Society, New York, NY, April 1986.
Sharon G. Lias

Activities of the Ion Kinetics and Energetics Data Center, Presentation at Workshop on Ion Thermochemistry, NATO ASI on Structure/Reactivity and Thermochemistry of Ions, Les Arcs, France, July, 1986
Sharon G. Lias

Future of Information Flow: Tertiary Information Providers, International Council for Scientific and Technical Information, York, England, May 1986
David R. Lide, Jr.

Numerical Databases, Industrial Technical Information Managers Meeting, Princeton, NJ, October 1986
David R. Lide, Jr.

National Standard Reference Database Series, CODATA '86 Conference, Ottawa, Canada, July 1986
Bettijoyce B. Molino

CODATA Referral Database, CODATA '86 Conference, Ottawa, Canada, July 1986
Bettijoyce B. Molino

Need for An ASTM Standards Development Activity, ASTM Committee E49 Organization Meeting, Philadelphia, PA, March 1986
John R. Rumble, Jr.

Near Future and Long-Range Goals Necessary for Meeting National Needs for Materials Property Data, 31st International Symposium of SAMPE, Las Vegas, NV, April 1986
John R. Rumble Jr.

Technical Data Bases on the International Scene - Trends and Issues, 31st International Symposium of SAMPE, Las Vegas, NV, April 1986
John R. Rumble, Jr. and D. R. Lide, Jr.

Databases in the Scientific and Technical Data Cycle, CODATA '86 Conference, Ottawa, Canada, July 1986
John R. Rumble, Jr.

Computerized Materials Property Data Systems, Proceedings, Oceans '86 Conference, Washington, DC, September 1986
John Rumble, Jr. and J. Gilbert Kaufman

Database Design, National Workshop on Computerization of Welding Data, Knoxville, TN, August 1986
John R. Rumble, Jr.

Technical Decision Making and Computers: An Overview, Annual Meeting of ASIS, Chicago, IL, October 2, 1986
John R. Rumble, Jr.

Goals for the Materials Data Interchange Format, Fall Meeting, ASTM Committee E49, Phoenix, AZ, October 1986
John R. Rumble, Jr.

Computerizing Materials Data - Challenges to the Ceramics Community, 39th Pacific Coast Regional Meeting of American Ceramic Society, Seattle, WA, October 1986
John R. Rumble, Jr.

Material Database Development, CODATA Workshop on Material Databases, Paris, France, November 1986
John R. Rumble, Jr.

EXHIBITS BY OSRD

191st ACS National Meeting and Exposition, New York, NY, April 13-16, 1986

192nd ACS National Meeting and Exposition, Anaheim, CA, September 7-12, 1986

TECHNICAL AND PROFESSIONAL COMMITTEE PARTICIPATION AND LEADERSHIP

Judith T. Calabrese

Bedford Composition System Users Group

Alice A. Dugan

NML Administrative Council

Sharon G. Lias

Member, Organizing Committee of NATO ASI on "Structure/Reactivity and Thermochemistry of Ions," June 29-July 11, 1986, in Los Ares, France

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

Member, Editorial Board of the NBS Journal of Research

David R. Lide, Jr.

American Institute of Physics (AIP Publication Board)

Committee on Nomenclature, ACS

Section Committee, Chemistry, AAAS

Journal of Physical and Chemical Reference Data (Editor)

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

International Union of Pure and Applied Chemistry (Member of Bureau, Chairman of Division Presidents Group)

Physical Chemistry Division, IUPAC (President)

Committee on Chemical Databases, IUPAC (Chairman)

U. S. National Committee for IUPAC

Advisory Council, Engineering Information, Inc.

Advisory Committee, Particle Data Center, Lawrence Berkeley Laboratory

Eighth International Conference on Computers in Chemical Research and Education (China, 1987) (Scientific Program Committee)

Workshop on Nucleic Acid and Protein Sequencing Data (Local Organizing Committee)

International Council for Scientific and Technical Information (Executive Committee)

Bettijoyce B. Molino

NBS User Committee for Scientific Computing

NBS Personal Computer Advisory Committee

NBS National Measurement Laboratory EEO Advisory Panel

NBS National Measurement Laboratory Performance Standards Review Board

ACS Division of Chemical Information (Treasurer)

ACS Committee on Science - Task Force on Scientific Numeric Data

CODATA Task Force on a Referral Database (Secretary)

Scientific Program Committee of the 11th International CODATA Conference (Germany, 1988)

ICSTI Numerical Data Group

Bedford Composition System Users Group

John R. Rumble, Jr.

Steering Committee, Aerospace Workshop on Computerized Materials Property and Design Data

ASTM Committee E-49 Computerized Materials Data (Vice-Chairman)

ASTM Committee E-42 Surface Analysis

Metal Properties Council Task Group of the National Materials Property Data Network
Chairman - User Needs Committee

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

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

Scientific Program Committee for the 10th International CODATA Conference (Canada, 1986)

Metals Information Committee of ASM

Constance L. Seymour

Bedford Composition Systems Users Group

Howard J. White, Jr.

International Association for the Properties of Steam (Executive Secretary)

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

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

Engineering Sciences Data Unit Ltd. (Corresponding Member)

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

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

American Petroleum Institute Subcommittee on Technical Data (Advisor)

Public Law 90-396
90th Congress, H. R. 6279
July 11, 1968

An Act

To provide for the collection, compilation, critical evaluation, publication, and sale of standard reference data.

Be it enacted by the Senate and House of Representatives of the United States of America in Congress assembled,

Standard Reference Data Act.

DECLARATION OF POLICY

SECTION 1. The Congress hereby finds and declares that reliable standardized scientific and technical reference data are of vital importance to the progress of the Nation's science and technology. It is therefore the policy of the Congress to make critically evaluated reference data readily available to scientists, engineers, and the general public. It is the purpose of this Act to strengthen and enhance this policy.

82 STAT. 339

DEFINITIONS

82 STAT. 340

SEC. 2. For the purposes of this Act—

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

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

Collection and publication of standard reference data.

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

Standards, etc. Publication in Federal Register.

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

Sale of reference data. Cost recovery.

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

31 Stat. 1449; Ante, p. 34.

U. S. copyright and renewal rights. 61 Stat. 655; 76 Stat. 446.

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

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

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

Appropriation.

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

Short title.

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

Approved July 11, 1968.

LEGISLATIVE HISTORY:

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

NSRDS DATA CENTERS

Alloy Phase Diagram Data Center

Dr. J. B. Clark
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National Bureau of Standards
Gaithersburg, MD 20899
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Aqueous Electrolyte Data Center

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National Bureau of Standards
Gaithersburg, MD 20899
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Atomic Collision Cross Section Data Center

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Joint Institute for Laboratory Astrophysics
University of Colorado
Boulder, CO 80309
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Atomic Energy Levels Data Center

Dr. W. C. Martin
Center for Radiation Research
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National Bureau of Standards
Gaithersburg, MD 20899
Telephone: (301) 975-3212

Atomic Transition Probabilities Data

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Center for Radiation Research
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Chemical Thermodynamics Data Center

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Chemistry Bldg. - Room A155
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Crystal Data Center

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National Bureau of Standards
Boulder, CO 80303
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Fundamental Constants Data Center

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*Fundamental Particle Data Center

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Molecular Spectra Data Center

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Molten Salts Data Center

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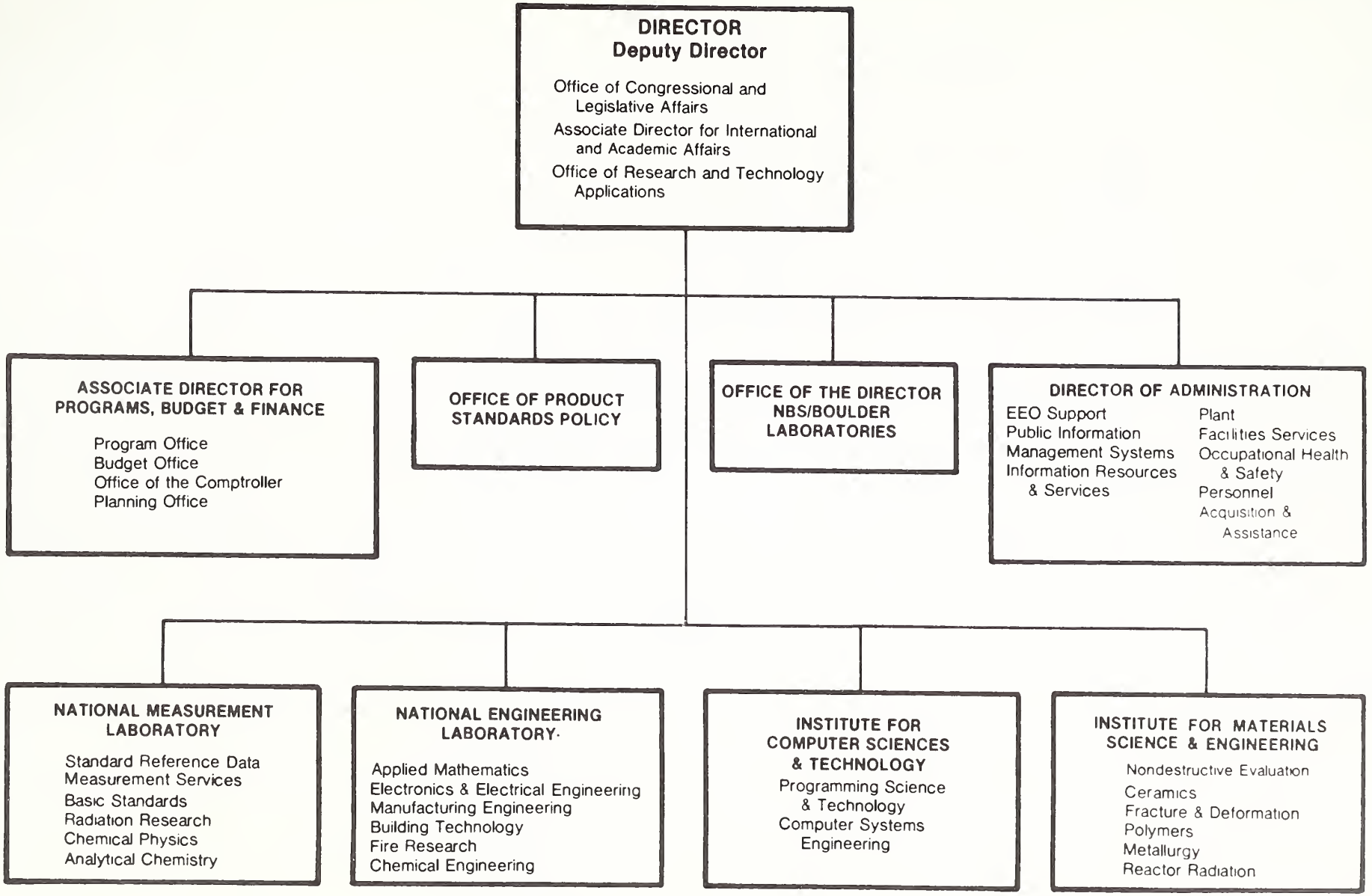
*The Office of Standard Reference Data is not involved at the present time in the administration or funding of these data centers but assists in making their outputs and services known to the scientific community.

U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards



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U.S. DEPT. OF COMM. **BIBLIOGRAPHIC DATA SHEET** (See instructions)	1. PUBLICATION OR REPORT NO. NBSIR 87-3526	2. Performing Organ. Report No.	3. Publication Date FEBRUARY 1987

4. TITLE AND SUBTITLE

Technical Activities 1986
Office of Standard Reference Data

5. AUTHOR(S)

David R. Lide

6. PERFORMING ORGANIZATION (*If joint or other than NBS, see instructions*)

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

7. Contract/Grant No.

8. Type of Report & Period Covered

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

10. SUPPLEMENTARY NOTES

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

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

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

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the program for the year 1986.

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 1986.

13. AVAILABILITY

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☐ Order From Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402.

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14. NO. OF PRINTED PAGES

15. Price