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Technical Activities 1980
Office of Standard Reference Data

S. P. Fivozinsky, Editor

National Measurement Laboratory
U.S. Department of Commerce
National Bureau of Standards
Washington, DC 20234

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PARTMENT OF COMMERCE
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U.S. DEPARTMENT OF COMMERCE, Malcolm Baldrige, *Secretary*
NATIONAL BUREAU OF STANDARDS, Ernest Ambler, *Director*

ABSTRACT

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

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the Program for the year 1980.

key words: data compilation, energy and environmental data, evaluated data, materials data, standard reference data, thermochemical and thermophysical data, technical activities 1980.

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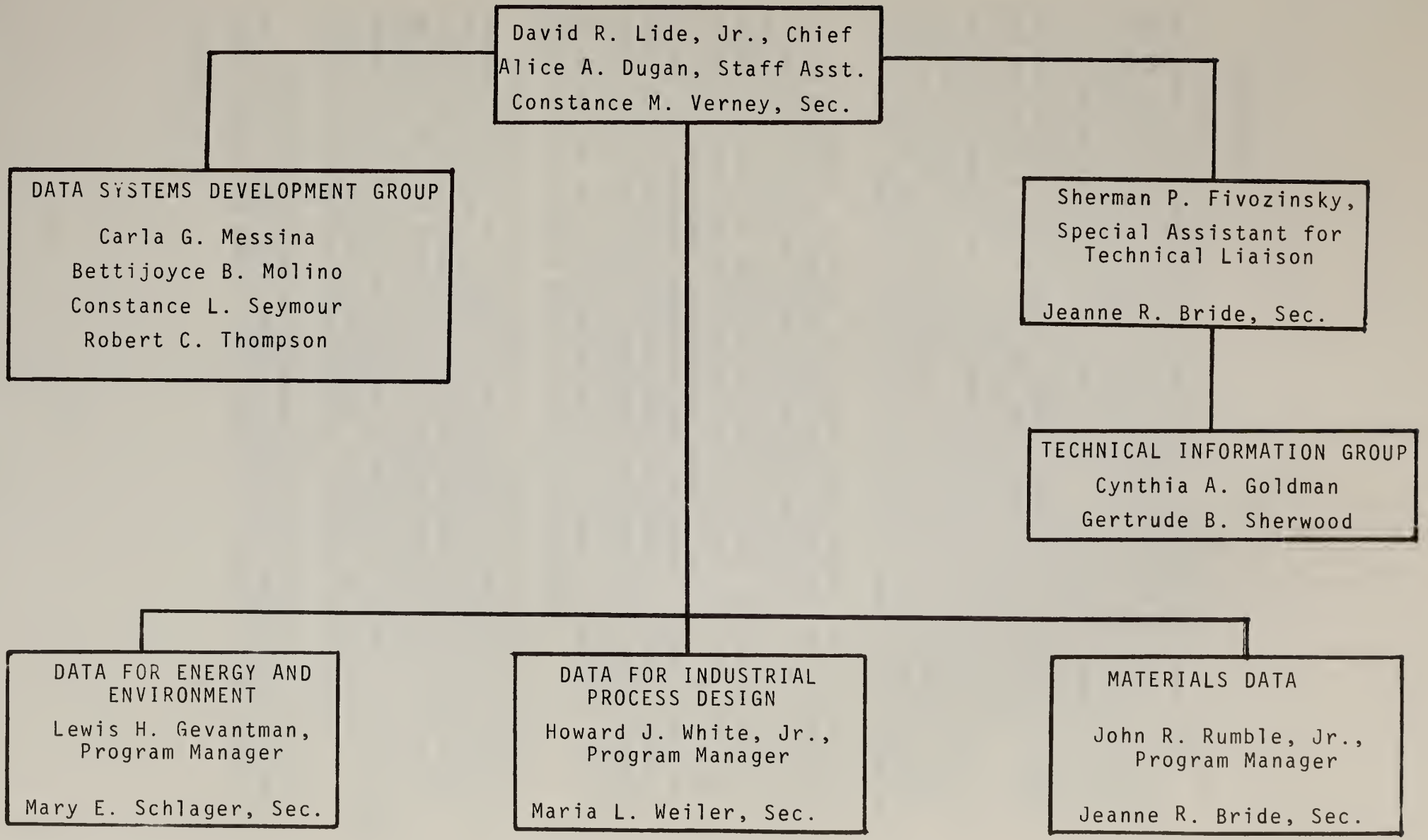


Introduction

The Office of Standard Reference Data is responsible for program management and coordination of the National Standard Reference Data System (NSRDS). The 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 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 an 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 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

*See Appendix B.

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.

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 a 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 selections of recommended values and accuracy estimates.

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

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

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

Appropriate publications of technical societies and commercial publishers.

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

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

Highlights of 1980 Activities

The publication of data compilations and critical reviews continued at a high level in 1980. Eighteen articles appeared in Volume 9 of the Journal of Physical and Chemical Reference Data, the primary output channel for the program. The circulation of this journal continues to increase slowly, during a period when most scientific journals are experiencing a gradual decline in subscriptions. In addition, five data publications appeared in the NSRDS-NBS series, and seven bibliographies and other publications came out in other NBS series. The year also saw the first issue of the Bulletin of Alloy Phase Diagrams, a joint publication of NBS and the American Society for Metals. Citations to NSRDS publications now run well above 2500 per year.

An important new undertaking of the Office of Standard Reference Data in 1980 was the establishment of an interagency program to support data evaluation projects in universities and industry. Initial support for the program has come from the National Science Foundation, Department of Energy, and Office of Naval Research, which transferred a total of $500,000 to OSRD in FY 1980 for this purpose. Over 40 proposals were received; eight grants have been made, and another five or six are expected to be processed by the end of 1980. We hope through this program to promote broader participation of the scientific community in data evaluation activities.

Cooperative activities with the private sector have also been expanded during the last year. An agreement was signed in May with the American Institute of Chemical Engineers which permits full OSRD participation in the Design Institute for Physical Property Data (DIPPR). This organization, which is supported by the chemical industry, has set up an ambitious program to provide design data for the chemical engineering community. Another agreement, with the American Society for Metals, covers an international program on alloy phase diagrams. The organization of this program is well along, and the first publications have already appeared.

Progress was made during the year on the development of computerized data bases and their dissemination to the public. Usage of the mass spectral data base, which is maintained by OSRD on the on-line Chemical Information System (CIS), has increased sharply. A single crystal data base is almost ready to install on the CIS, and software development has been started which will handle various thermodynamic data bases. A comprehensive study of the formats of both bibliographic and numerical data bases maintained in NSRDS data centers is underway, with the objective of bringing the less automated centers up to the level of the others.

Three new thrusts for the Standard Reference Data Program were pursued in the FY 1982 budget cycle. A proposal for a major expansion of work on fluid properties was incorporated into a broader NBS initiative on chemical engineering. This has been approved at the Department of Commerce level and is now being considered by OMB. Initiatives on data related to ionizing radiation and on computer dissemination of SRD were approved by the Director of NBS but did not survive the screening at the Department of Commerce. However, as a result of the presentation of these initiatives, OSRD expects to receive funds from the Director's reserve in FY 81 to begin the proposed work on fluid properties and computerization.

Reports of Standard Reference Data Tasks

The activities of the Standard Reference Data program are organized under seven application-oriented tasks. The first of these tasks includes the management, coordination, and dissemination functions of the Office of Standard Reference Data. Three tasks deal with data centers and other projects whose output is particularly relevant to energy and environmental problems. Two tasks cover activities in the general area of thermodynamics and physical properties relevant to industrial process design, with a particular focus on the chemical industry. The final task includes properties of structural materials, especially those which influence materials durability and performance. A summary of progress on each of these tasks is given in this section.

TASK NUMBER: 14401
TITLE: NSRDS Coordination and Dissemination
LEADER: Lide, D. R., Jr.
TASK OBJECTIVE: Coordinate the activities of the National Standard Reference Data System, including both NBS projects and those at universities, Government laboratories, and industrial establishments; maintain liaison with other U.S. and foreign institutions concerned with reference data so as to avoid duplication and assure optimum coverage; establish criteria for evaluation and presentation of data; disseminate reliable reference data to the scientific and engineering community through appropriate mechanisms tailored to user needs.

ACTIVITY CATEGORIES: Management and Coordination
Publications
Technical Liaison and Information Service
Data Systems Development

TASK STATUS: Many of the activities in this overall management task are covered elsewhere in the report. The publication and dissemination function represents a large part of the work of this task. Publications issued in 1980 are listed under the programmatic task with which they are associated. The following tables summarize the published output of the program and the distribution of this output:

Publications in 1980

Series	Pages Published	Titles Published
JPCRD, Vol. 9	1350	18
NSRDS-NBS	3160	5
Data Compilations in other NBS series	661	3
Data Compilations from other publishers	813	3
Bibliographies and Indexes in NBS series	478	4
Bibliographies and Indexes from other publishers	2274	4
Totals	8736	37

Subscribers to JPCRD

Month/Year	Number
9/1977	1156
9/1978	1205
9/1979	1237
9/1980	1234

Inquiries Received in OSRD

(Does not include inquiries received by data centers.)

Year	Number
1977	530
1978	730
1979	882
1980*	840

Sales of JPCRD Offprints and Supplements

Year	Offprints	Supplements
1977	4078	567**
1978	5577	184
1979	5981	137
1980*	5079	111

* Projected to end of year.

** New supplement issued in 1977.

A number of other accomplishments in 1980 are worthy of mention:

- A computer-based indexed file of NSRDS outputs is nearing completion. Materials, property, and author indexes for the Journal of Physical and Chemical Reference Data have been assembled this year using the system. The typesetting tape for the indexes is produced directly from the system software. The complete NSRDS Publication List with indexes will be produced from the new file.

- The results of a study of the NBS role in nuclear waste management has led to DOE funding of a comprehensive program through the NBS Office of Measurements for Nuclear Technology. This program will include funding for reference data activities on phase diagrams of ceramics, powder diffraction patterns, and geologic properties.

- The OSRD was a supporter of the Symposium on High Resolution Infrared Applications and Developments, held at NBS June 23-25, 1980.

- The OSRD was host to the Chemical Information System Steering Committee and to its newly established Scientific Advisory Board.

- OSRD staff have been heavily involved in organizing the 7th International CODATA Conference. Two staff members presented papers.

- A summary of on-line or interactive physico-chemical numerical data systems is being published (Hilsenrath, Technical Note 412).

- Data Handling for Science and Technology, An Overview and Source-book, is being published by North Holland (S. A. Rossmassler and D. G. Watson, Editors).

- Two chapters of a major listing of data sources are being edited by OSRD staff (D. R. Lide and L. H. Gevantman). The completed work will be published by CODATA.

The OSRD continues active participation in the planning of data programs of national and international bodies, such as the American Institute of Chemical Engineers (AIChE), the American Association of Physicists in Medicine (AAPM), the Committee on Data for Science and Technology (CODATA), the International Union of Pure and Applied Chemistry (IUPAC), and the International Association for the Properties of Steam (IAPS).

TASK NUMBER: 14420
TITLE: Physical Data for Energy Applications
LEADER: Gevantman, L. H.
TASK OBJECTIVE: Provide the scientific and engineering community with physical property data relevant to the more effective utilization of energy and the development of new energy sources; maintain the primary data bases required for the analysis of energy options; develop the capability for preparing sets of critically evaluated data needed in specific energy R & D programs.

TASK NUMBER: 14425 (Other Agency)
TITLE: Data for Energy Systems Applications and Design
LEADER: Gevantman, L. H.
TASK OBJECTIVE: Compile, evaluate, and disseminate physical and engineering properties data required for specific applications to systems for energy production, storage, and conservation. Disseminate the data to the user, employing distribution media such as books and journal publication, magnetic tape, accessible automated data files, etc.

DATA CENTERS:

Atomic Energy Levels Data Center (Atomic and Plasma Radiation Division, Center for Radiation Research, NBS) - Spectra and energy levels for atoms and ions.

Atomic Transition Probabilities and Line Shapes and Shifts Data Center (Atomic and Plasma Radiation Division, Center for Radiation Research, NBS) - Atomic transition probabilities, spectral line shapes and oscillator strengths for atoms and ions.

X-ray and Ionizing Radiation Data Center (Radiation Physics Division, Center for Radiation Research, NBS) - Photon cross sections and mass attenuation coefficients for the elements; cross sections for photoabsorption, coherent and incoherent scattering, pair and triplet production.

Photonuclear Data Center (Nuclear Radiation Division, Center for Radiation Research, NBS) - Evaluated photonuclear cross section data for reactions of interest; giant resonances, excitation energies, and angular distribution.

Atomic Collision Cross Section Data Center (Quantum Physics Division, Center for Absolute Physical Quantities, NBS) - Low-energy collision cross section data for electrons and photons with atoms and molecules; transport properties, including electron swarm data, electron affinities, and plasma conductivity.

Molten Salts Data Center (Rensselaer Polytechnic Institute, Troy, New York) - Transport and thermodynamic properties including viscosity, surface tension, electrical conductivity, density, and phase diagrams.

DATA CENTERS: (continued) Chemical Kinetics Information Center (Chemical Kinetics Division, Center for Thermodynamics and Molecular Sciences, NBS) - Chemical kinetic rate constant data on elementary gas phase reactions; photochemical rate data.

TASK STATUS: As reported previously, the two tasks are served by the same data centers. Their activities under these tasks are directed toward improving the state of knowledge in fields concerned with energy production and application, such as nuclear reactor technology, magnetic and laser fusion, fossil fuel combustion, energy conservation and storage, and solar energy.

Again, goals for progress toward realizing nuclear fusion for power were emphasized. A number of publications on atomic energy levels data and atomic and molecular collision data highlighted the output in this area. Further interaction with the IAEA Atomic and Molecular Data section resulted in a solidification of IAEA plans to merge and disseminate numerical data inputs from all over the world.

A reprogramming effort is presently under way to widen the scope of the nuclear data center objectives to include photon and particle interactions with all matter. Thus, in addition to their applicability to the area of nuclear power production, these data activities will also encompass radiation effects on material improvement. The data will also apply to problems encountered in the areas of radiation health and safety. Relative to the above, the Photonuclear Data Center is now in the final stages of preparing a manuscript on reaction data for carbon, nitrogen, and oxygen.

The data book on rock salt properties aimed at the design of nuclear waste isolation facilities is now in the final stages of publication and should issue by the end of the calendar year. The feasibility study on the availability of physical properties data on granite, basalt, shale, and tuff is being actively pursued and is nearing completion. Depending on its outcome new data projects to evaluate similar data for these materials will be established.

Continued efforts to elucidate hydrocarbon combustion kinetics with a view toward improved efficiencies have resulted in the issuance of evaluated tables of kinetic rates on over 100 reactions. Nine more data sheets, for a total of fifteen, on high temperature reaction rate data are being readied, and a manuscript documenting the evaluative effort and its output to date is being prepared.

The data compilation project on materials used in energy storage and conservation is nearing completion with the coming publication of data on new molten salt mixtures. Only data on polymer matrix materials remains to be completed before this project can be considered concluded. Other data projects involving electrochemical processes either for energy storage or conservation have experienced some publication delay.

PUBLICATIONS IN 1980:

Energy Levels of Magnesium, Mg I through Mg XII, W. C. Martin and Romuald Zalubas, JPCRD Vol. 9, No. 1, pp. 1-58.

Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion, Francis Westley, NSRDS-NBS 67.

Energy Levels of Scandium, Sc I through Sc XXI, Jack Sugar and Charles Corliss, JPCRD Vol. 9, No. 2, pp. 473-512.

Pair, Triplet and Total Atomic Cross Sections and Mass Attenuation Coefficients for 1 MeV - 100 GeV Photons in Elements Z = 1 to 100, J. H. Hubbell, H. A. Gimm, and I. Øverbø, JPCRD Vol. 9, No. 4.

Physical Properties Data for Rock Salt, L. H. Gevantman, Editor, NBS Monograph 167.

A Compilation of Kinetic Parameters for the Thermal Degradation of n-Alkane Molecules, D. L. Allara and R. Shaw, JPCRD Vol 9, No. 3, pp. 523-560.

Molten Salts Reference Standards for Density, Surface Tension, Viscosity, and Electrical Conductance: KNO_3 and NaCl, G. J. Janz, JPCRD Vol. 9, No. 4.

Molten Salts: Volume 5, Part 1. Additional Single and Multi-Component Salt Systems. Electrical Conductance, Density, Viscosity, and Surface Tension Data, G. J. Janz and R. P. T. Tomkins, JPCRD Vol. 9, No. 4.

Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, O v, C. E. Moore NSRDS-NBS 3, Section 9.

Tables of Line Spectra of the Elements. Part 1, Wavelengths and Intensities. Part 2, Transition Probabilites, J. Reader, C. H. Corliss, W. L. Wiese, and G. A. Martin, NSRDS-NBS 68.

Bibliography on Atomic Transition Probabilities (November 1977 through March 1980), B. J. Miller, J. R. Fuhr, and G. A. Martin, NBS Spec. Publ. 505-1.

Bibliography of Low Energy Electron Cross Section Data (1978), J. W. Gallagher and E. C. Beaty, JILA Information Center Report No. 18.

PUBLICATIONS IN 1980: (continued) Bibliography on Atomic Energy Levels and Spectra, July 1975 through June 1980, R. Zalubas and A. Albright, NBS Spec. Publ. 363, Supplement 2.

TASK NUMBER: 14430
TITLE: Reference Data for Environment and Health
LEADER: Gevantman, L. H.
TASK OBJECTIVE: Compile, evaluate, and disseminate physical and chemical properties data on substances impacting the environment, with primary emphasis on those causing undesirable changes in man's surroundings or affecting human health; provide the necessary data bases for the identification of such substances and for the prediction of their transport, transformation, and ultimate fate in the environment.

DATA CENTERS: Molecular Spectra Data Center (Molecular Spectroscopy Division, Center for Thermodynamics and Molecular Science, NBS) - Microwave and infrared spectra of gaseous molecules; frequencies, intensities of absorption spectra; molecular constants.

Ion Energetics Data Center (Chemical Thermodynamics Division, Center for Thermodynamics and Molecular Science, NBS) - Heats of formation of gaseous ions; appearance and ionization potentials; proton affinities.

Chemical Kinetics Information Center (Chemical Kinetics Division, Center for Thermodynamics and Molecular Science, NBS) - Gaseous reaction rate constants for elementary reactions, photochemical rate constants, activation energies for gaseous elementary reactions.

Radiation Chemistry Data Center (Radiation Laboratory, University of Notre Dame, Notre Dame, Indiana) - Reaction rate constants for ionizing and photochemical interactions with aqueous and other liquid media; G factors, radical yields, radical spectra and lifetimes.

Aqueous Electrolyte Data Center (Chemical Thermodynamics Division, Center for Thermodynamics and Molecular Science, NBS) - Activity and osmotic coefficients of inorganic salts in aqueous media.

TASK STATUS: The identification and quantification of environmental pollutants remains a serious problem. The traceability of these substances and knowledge of their interactions with other materials in the biosphere prior to their being rendered harmless constitutes a prime effort. As a consequence the need arises for data to detect, identify, and track these substances present in highly dilute concentrations. Many of the efforts described in this task are devoted to the buildup of a body of data which would help in the solution of environmental pollution. They relate particularly to spectral measurements inasmuch as such techniques provide the necessary sensitivities required.

The Molecular Spectra Data Center continues to issue microwave spectral data on such molecules as formic acid, methyl cyanide, and others. In addition, data on the fundamental vibrational frequencies of halogenoalkanes and halogenoalkyl ethers have been issued in collaboration with scientists in Japan.

The EPA/NIH mass spectra data file is disseminated in two forms. The data tape is leased by 31 organizations resident in eight countries, including the United States. The book form has been reprinted to accommodate the continued demand for the hard-copy form, and a Supplement containing over 8000 additional spectra is in the final stages of publication. In order to increase coverage of the literature and increase the number of quality spectra in the collection, the Office of Standard Reference Data (OSRD) has contracted with the Mass Spectral Data Centre, now at the University of Nottingham (England), to collect, evaluate, and enter new spectra into the data file. The estimated number of additional data is anticipated to average 1500 new spectra per year.

Consideration has been given to the automation and retrieval of other types of spectral data. A feasibility study, aimed at codification and ultimate digitization of IR spectra, has recently been completed under the aegis of the Joint Committee on Atomic and Molecular Physical Data (JCAMP) contracted jointly by OSRD and the Canadian National Research Council. A representative sampling of IR spectra is being digitized to establish a basic cost figure per spectrum. An interagency agreement with the Environmental Protection Agency (EPA) is also being negotiated to further this effort.

Data on the solubility of toxic metals in water have been published. They involve compounds of lead and mercury. In addition, the project on vapor pressure data (Henry's Law Constants) is nearing completion. Other data efforts aimed at elucidating the behavior of toxic substances in water will be considered. A related effort dealing with the solubility of chemical substances in a variety of solvent media is under way through the IUPAC's Commission V.8. This group has published two additional volumes, one dealing with the solubility of argon, and the other with the solubility of IA halides in amides.

Data for modelling pollutant reactions and ultimate fate of undesirable substances in the upper atmosphere have been improved by the report issued by the CODATA Task Group on Chemical Kinetics. Another group has submitted a manuscript to OSRD dealing with lower atmosphere evaluated kinetic data. Together they cover the present state-of-knowledge concerning atmospheric reactions. The outputs of the Radiation Chemistry Data Center extend the kinetic data into solution phase where a coming publication will deal with a compilation of aliphatic radical reaction rate constants in aqueous solution. The Ion Energetics Data Center has updated and published data on ionization and appearance potentials through 1973. In addition, the Center hopes to be completely up to date in the coming year (1981). These data

have implications not only in the environmental area but also in the fundamental processes involved in hydrocarbon combustion.

Finally, the published Annual Report of the Council on Environmental Quality (CEQ) has been well received. The task manager (L. H. Gevantman) made a contribution to the analysis of the trends and conditions of the national water quality.

PUBLICATIONS IN 1980:

Microwave Spectra of Molecules of Astrophysical Interest. XVIII. Formic Acid, E. Willemot, D. Dangoisse, N. Monnanteuil, and J. Bellet. JPCRD Vol. 9, No. 1, pp. 59-160.

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry, D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr, J. Troe, and R. T. Watson, JPCRD Vol. 9, No. 2, pp. 295-471.

The Solubility of Some Sparingly Soluble Lead Salts: An Evaluation of the Solubility in Water and Aqueous Electrolyte Solution, H. L. Clever and F. J. Johnston, JPCRD Vol. 9, No. 3, pp. 751-784.

Compilation and Evaluation of Solubility Data in the Mercury (I) Chloride-Water System, Y. Marcus, JPCRD Vol 9, No. 4.

Microwave Spectra of Molecules of Astrophysical Interest. XIX. Methyl Cyanide, D. Boucher, J. Burie, A. Bauer, A. Dubrulle, and J. Demaison, JPCRD Vol. 9, No. 3, pp. 659-720.

Tables of Molecular Vibrational Frequencies, Part 10, T. Shimanouchi, H. Matsuura, Y. Ogawa, and I. Harada, JPCRD Vol. 9, No. 4.

Ion Energetics Measurements, Supplement I. 1971-1973, H. M. Rosenstock, D. Sims, S. S. Schroyer, W. J. Webb. NSRDS-NBS 66.

EPA/NIH Mass Spectral Data Base, Supplement I and Cumulative Index, S. R. Heller and G. W. A. Milne, NSRDS-NBS 63 Supplement.

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Volume 12, 1979, Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame, Notre Dame, IN 64556.

PUBLICATIONS IN 1980: (continued)

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Volume 13, 1980, Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame, Notre Dame, IN 46556.

Chemical Kinetic and Photochemical Data Sheets for Atmospheric Reactions, R. F. Hampson, Jr., U. S. Department of Transportation, Federal Aviation Administration, Report No. FAA-EE-80-17.

Projects supported by OSRD have made contributions to the following publications:

CEQ Annual Report

IUPAC Solubility Data Series, Pergamon Press

Argon, H. L. Clever

IA-Halides in Amides, M. Salomon

TASK NUMBER: 14440
TITLE: Thermochemical Data for Process Design
LEADER: White, H. J., Jr.
TASK OBJECTIVE: Provide the chemical process and related industries with critically evaluated thermodynamically compatible data which can be used to establish the equilibrium constants and heats of reaction for all important chemical reactions; provide data describing the change in the chemical properties of substances with changes in temperature and at phase-transition points; provide bibliographic reference services on thermochemistry.

DATA CENTERS: Chemical Thermodynamics Data Center (Chemical Thermodynamics Division, Center for Thermodynamics and Molecular Science, NBS) - Enthalpies and Gibbs energies of formation, entropies and Cp in the standard state at 298.15 K and 1 atm.; enthalpies of formation at 0 K for inorganic substances and simple organic substances; transition properties; thermal functions.

Aqueous Electrolyte Data Center (Chemical Thermodynamics Division, Center for Thermodynamics and Molecular Science, NBS) - Thermodynamic properties of aqueous electrolyte solutions including activity and osmotic coefficients, excess and partial molal properties of solution, solubilities and equilibrium constants in solution.

Thermodynamics Research Center (Texas A&M University, College Station, Texas) - Thermodynamic properties of organic materials, condensed-phase properties, transition points and properties, density and vapor pressure of liquids, ideal gas and real gas properties.

TASK STATUS: The publication of NBS Technical Note 270-8 closes a series that started with Technical Note 270-1 published in 1965. The length of the task arose from two factors; the sheer bulk of the data array covered, approximately 12,000 individual entries, and the fact that the nature of the tables demands thermodynamic compatibility among the entries. The tables give enthalpies and Gibbs energies of formation for the elements and, as is well known, these can be combined to give the enthalpies and Gibbs energies of reactions involving the compounds in the tables. The compatibility requirement arises from the fact that any set of reactions that can be reduced to the same net reaction, for example, all possible methods to separate water into H_2 and O_2, must give identical values for the enthalpy or Gibbs energy of the net reaction. Initially compatibility was introduced by careful iterative hand procedures. As the task proceeded computerized methods for the solution of large arrays of simultaneous equations and for showing the primary interrelationships between substances were developed. These enabled the compatibility to be introduced by computerized means. The automation of the introduction of thermodynamic compatibility will completely alter the production of future tables of this type by allowing many more workers to participate in the initial steps and reducing the introduction of compatibility to a series of computer runs.

The provision of data on the osmotic and activity coefficients of aqueous electrolyte systems has continued. At the present time all available data for the 2:1 and 1:2 valence classes of substances at 25°C have been evaluated. Papers covering these classes have either been published or are in various stages of the publication process.

The data file for the TN 270 series has been automated and is in the process of being entered into the Chemical Information System (CIS). CIS is an on-line interactive data system that is accessible to subscribers by telephone line.

PUBLICATIONS IN 1980:

Selected Values of Chemical Thermodynamic Properties: Compounds of Uranium, Protactinium, Thorium, Actinium and the Alkali Metals, D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm and R. L. Nuttall, NBS Technical Note 270-8.

Tentative Set of Key Values for Thermodynamics, Part 8. prepared by the CODATA Task Group on Key Values for Thermodynamics, CODATA.

The Thermochemical Properties of the Uranium-Halogen Containing Compounds, V. B. Parker, NBS IR80-2029,

Bulletin of Chemical Thermodynamics, Vol. 23, 1980, IUPAC Commission on Thermodynamics and Thermochemistry, Robert D. Freeman, Editor.

TASK NUMBER: 14450
TITLE: Thermophysical Data for Process Design
LEADER: White, H. J., Jr.
TASK OBJECTIVE: Provide industry with standard reference data on the thermodynamic and transport properties of single substances and non-reacting mixtures of substances as functions of temperature, pressure, and relative proportions of components, by critical evaluation of existing experimental data, and by utilization of evaluated calculation techniques to interpolate and extrapolate over ranges of variables and to estimate data.

DATA CENTERS: Cryogenic Data Center (Thermophysical Properties Division, Center for Mechanical Engineering and Process Technology, NBS) - Thermophysical properties of cryogenic fluids and their mixtures, properties of materials of construction for cryogenic systems.
Thermodynamic Research Laboratory (Washington University, St. Louis, Missouri) - Vapor-liquid equilibrium, excess enthalpy and excess volume of binary sub-critical fluid mixtures, vapor pressures, real gas properties of single component fluids.
CINDAS (Purdue University, West Lafayette, Indiana) - Thermal and electrical conductivities of metals and alloys, viscosities, thermal conductivities, heat capacities of industrially important fluids.

TASK STATUS: This Task emphasizes the thermophysical properties of fluids (and, to a lesser extent, solids) which are required in a wide variety of engineering problems. These data enter, for example, into the design of heat exchangers, compressors, turbines, and similar equipment which employ fluids; they are key elements in separation processes such as distillation; and they are needed for reliable metering of fluids transferred through pipelines. The ability to predict the properties of fluid mixtures from the pure fluid data is important, since mixtures are the normal rule in most industrial processes.

The abundance of water which characterizes our planet assures it a unique place in our technology. Water is probably the most extensively studied chemical substance and the one for which reference data are needed most frequently and for the most widely varying purposes. A coordinated program of study of the thermodynamic properties of water has resulted in the first three publications listed below.

The work leading to each of these publications required new technical developments before the reference data could be prepared. The preparation of the data on the ideal-gas properties required a more detailed consideration of excited states for water than had been done before. The data in the critical region required the use of scaling-law techniques to develop an expression for a state function, the Helmholtz energy, so that the data for several different

properties would be thermodynamically compatible. The formulation for the properties in the classical region was required to cover a wider range of temperatures and a much wider range of pressures than had been covered before. This problem was solved by a new technique building the formulation on a single physically-based model for the high-density fluid. As a result, the formulation is relatively simple in regions of high density and shows physically-realistic behavior on extrapolation.

Emphasis on the properties of mixtures was increased during 1980 with an increase in analysis of the methods available for treating mixtures. A further paper on mixtures is listed below. In addition the popular bibliographic source, Equilibrium Properties of Fluid Mixtures, by Hiza Kidnay and Miller has been extended and updated and is ready for publication.

Difficulties in treating the region near the critical point have delayed the completion of the work on ethylene. A final report on this work is in preparation but some additional work is desirable and hopefully can be carried out.

PUBLICATIONS IN 1980:

Thermodynamic Properties of Fluid Water, L. Haar, J S. Gallagher and G. S. Kell pg. 69-83 in Water and Steam: Their Properties and Current Industrial Applications: Proceedings of the 9th International Conference on the Properties of Steam held at the Technische Universität München, FRG, 10-14 Sept. 1979, J. Straub and K. Scheffler Editors, Pergamon Press.

A Revised and Extended Scaled Fundamental Equation for the Thermodynamic Behavior of Steam in the Critical Region, F. W. Balfour, J. V. Sengers, J. M. H. Levelt Sengers, pg. 128-138 in Water and Steam: Their Properties and Current Industrial Applications: Proceedings of the 9th International Conference on the Properties of Steam held at the Technische Universität München, FRG, 10-14 Sept. 1979, J. Straub and K. Scheffler Editors, Pergamon Press.

Thermodynamic Properties of H_2O in the Ideal Gas State, H. W. Woolley, pg. 158-166 in Water and Steam: Their Properties and Current Industrial Applications: Proceedings of the 9th International Conference on the Properties of Steam held at the Technische Universität München, FRG, 10-14 Sept. 1979, J. Straub and K. Scheffler Editors, Pergamon Press.

A Review, Evaluation and Correlation of the Phase Equilibria, Heat of Mixing and Change in Volume on Mixing for Liquid Mixtures of Methane & Propane, R. C. Miller, A. J. Kidnay, and M. J. Hiza, JPCRD Vol. 9, No. 3, pp. 721-734.

PUBLICATIONS IN 1980: (continued)

LNG Materials & Fluids, A User's Manual of Property Data in Graphic Format, Second Supplement, Douglas Mann, Editor, Cryogenics Division, NBS, Boulder, CO.

An Improved Representative Equation for the Dynamic Viscosity of Water Substance, J. T. R. Watson, R. S. Basu, and J. V. Sengers, JPCRD Vol. 9, No. 4.

Other publications of the NBS Cryogenic Data Center:

CDC Current Awareness Service - Biweekly;
Superconductivity Devices and Materials - Quarterly;
Liquified Natural Gas - Quarterly;
Hydrogen - Future Fuel - Quarterly.

TASK NUMBER: 14470
TITLE: Materials Durability and Resource Recovery Data
LEADER: Rumble, J. R.
TASK OBJECTIVE: To provide needed physical, chemical, and metallurgical data for a better understanding of the phenomena and processes involved in the performance of solid materials in use, and in recovery of available thermal energy from selected groups of such materials after original use.

DATA CENTERS: Alloy Data Center (Metallurgy Division, Center for Materials Science, NBS) - Evaluated phase diagram data for binary and multicomponent alloys; related thermodynamic and physical properties data.

Crystal Data Center (Ceramics, Glass, and Solid State Division, Center for Materials Science, NBS) - Crystallographic data: cell parameters and ratios, space group, number of formula units per cell, density, etc., on inorganic and organic compunds, including metals, intermetallics, and minerals.

Diffusion in Metals Data Center (Metallurgy Division, Center for Materials Science, NBS) - Data on condensed-state diffusion and mass-transport phenomena involving all substances as the diffusing material, and all metal and alloy systems as the matrix.

Phase Diagrams for Ceramists (Ceramics, Glass, and Solid State Division, Center for Materials Science, NBS) - Evaluated phase diagrams of oxides, halides, cyanides, sulfides, etc., and their binary, ternary, and higher order systems.

TASK STATUS: Work under this task seeks improvements in the productivity of research and the effectiveness of technology in selected areas of materials performance in use and materials recovery after use. In particular, data compilation and evaluation efforts address the characterization of corrosion products, the analysis of corrosion processes, the identification of wear debris, and other areas related to materials durability. Diffusion and mass transport data are analyzed to provide better understanding of how corrosive substances diffuse into and affect structural materials. Phase stability data are systematically evaluated, and new methods devised for their prediction, presentation, and application in the development and design of new alloy, ceramic, and metallic/non-metallic systems.

All the data centers compile, maintain, evaluate, and disseminate comprehensive indexed collections of references and data relating to each center's area of interest. The resulting bibliographic and numerical data bases naturally form the basic resources used by the centers as they address various data problems and requests.

The task on Materials Durability and Resource Recovery has increased its activities since the reprogramming described in the 1978 OSRD Annual Report as reflected in the following activities of the data centers and other projects.

The Alloy Data Center is presently evaluating phase stability data and phase diagrams for all binary alloys containing titanium and one other element. These systems are of current interest for many reasons, especially for their use in light-weight heat-resistant fabricated products, as substitutes for durable stainless-steel chromium alloys, and as a high-strength material for underwater vessels. In addition, the joint NBS/American Society of Metals International program on alloy phase diagram data continues with important progress being made in two areas. The new periodical "Bulletin of Alloy Phase Diagrams" has been published. This journal will be a major source of evaluated phase diagrams to the user community and represents an important step in updating of the available data. The other major area of progress has been in the automation of storing, recalling, and manipulating phase diagrams. Work to date provides a solid foundation for theoretical modelling efforts, easier dissemination, and reliable presentation of phase diagrams.

Currently, the Diffusion in Metals Data Center is especially concerned with the evaluation of data relating to mass transport and diffusion phenomena in the durability of copper and its alloys, particularly multicomponent alloys. These systems are of great interest with respect to understanding and avoiding corrosion problems. This work is sponsored in part by the International Copper Research Association (INCRA) and will result in the second volume of evaluated data on these subjects pertaining to copper systems. The Data Center has continued its close interaction with the industrial community, acting as the primary source of evaluated data in all alloy diffusion areas.

The Alloy Data Center and the Diffusion in Metals Data Center have completed, in the past year, a major compilation and evaluation of data for candidate hydrogen storage materials. Data sheets covering eighteen possible physical and chemical properties, including reaction rates, diffusion coefficients, and phase diagrams have been prepared for Lawrence Livermore Laboratory where an on-line data base for these materials is being established.

The Crystal Data Center is in the final stages of completion of the new Crystallographic Identification File. This file contains information on over 57,000 crystalline compounds including microcontaminants, corrosion products, and metals needed for single crystal identification. The file will be of much importance to industrial laboratories and other research efforts, and will be of special value in reducing duplicate measurements. The Data Center plans to distribute the file through the on-line Chemical Information System and the Cambridge University network of Affiliated Crystal Data Centres.

The Crystal Data Center has also completed an intensive user evaluation of its products and services. The results indicate a high usage of Crystal Data, a joint NBS-JCPDS publication, with particular applications to materials analysis and design. Suggestions are being incorporated into the Data Center work to better serve the user community. The Data Center has developed a program (NBS*AIDS80) for the computer-assisted evaluation of crystallographic data. This project was done jointly with the JCPDS. Aside from the obvious use as a tool in the creation and manipulation of large data files, the program has already found great utility in analyzing published data for consistency and accuracy. It is hoped that this will facilitate the finding and correcting of errors by research scientists and journal editors prior to publication.

The Phase Diagrams for Ceramists Data Center has recently sent to publication volume four in the series "Phase Diagrams for Ceramists." This volume contains evaluated phase diagram data on metals, oxygen, and metal oxides, and continues the tradition of NBS as the major source of such evaluated systems. As the capability to design new materials with predicted properties has grown, the need for accurate phase diagram information for systems of metals with non-metallic components has increased correspondingly.

The Diffusion in Polymers Project is near completion on a comprehensive review of diffusion constants of organic molecules in polyolefins. This review will, for the first time, provide an accessible and complete source of these data. With increased interest in the diffusion into and out of plastics used as food-packaging material and countless other routine uses of plastics, such a data source will prove to be invaluable.

PUBLICATIONS IN 1980:

Phase Diagrams for Ceramists, Volume 4, R. S. Roth, L. P. Cook, and T. Negas, Editors, The American Ceramic Society.

Interactive Computer Graphics for Phase Diagram Storage, J. L. Murray, Bull. Alloy Ph. Diag. 1, No. 1.

Registration/Identification of Crystalling Materials Based on Lattice and Empirical Formula, J. Rodgers and A. D. Mighell, J. Chem. Inf. Comp. Sci. (in press).

User Evaluation of Crystal Data Products and Services, Questionnaire Analysis and Impact, J. K. Stalick, A. D. Mighell, and R. J. Boreni, NBS Technical Note 1112.

NBS*AIDS80, A Fortran Program to Evaluate Crystallographic Data, C. R. Hubbard, J. K. Stalick, and A. D. Mighell, Advances in X-ray Analysis, Plenum Press.

Publications in 1980

Journal of Physical and Chemical Reference Data, Volume 9

Energy Levels of Magnesium, Mg I through Mg XII
W. C. Martin and R. Zalubas

Microwave Spectra of Molecules of Astrophysical Interest. XVIII. Formic Acid
E. Willemot, D. Dangoisse, N. Monnanteuil, and J. Bellet

Refractive Index of Alkaline Earth Halides and Its Wavelength and Temperature Derivatives
H. H. Li

Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry
D. L. Baulch, R. A. Cox, R. F. Hampson, Jr., J. A. Kerr, J. Troe, and R. T. Watson

Energy Levels of Scandium, Sc I through Sc XXI
J. Sugar and C. Corliss

Comments: Revised Values of the Osmotic Coefficients and Mean Activity Coefficients of Sodium Nitrate in Water at 25 °C
Y. C. Wu and W. J. Hamer

A Compilation of Kinetic Parameters for the Thermal Degradation of n-Alkane Molecules
D. L. Allara and R. Shaw

Refractive Index of Silicon and Germanium and Its Wavelength and Temperature Derivatives
H. H. Li

Microwave Spectra of Molecules of Astrophysical Interest. XIX. Methyl Cyanide
D. Boucher, J. Burie, A. Bauer, A. Dubrulle, and J. Demaison

A Review, Evaluation, and Correlation of the Phase Equilibria, Heat of Mixing, and Change in Volume on Mixing for Liquid Mixtures of Methane + Propane
R. C. Miller, A. J. Kidnay, and M. J. Hiza

Saturation States of Heavy Water
P. G. Hill and R. D. Chris MacMillan

The Solubility of Some Sparingly Soluble Lead Salts: An Evaluation of the Solubility in Water and Aqueous Electrolyte Solution
H. Clever and F. J. Johnston

Molten Salts Reference Standards for Density, Surface Tension, Viscosity, and Electrical Conductance: KNO_3 and NaCl
George J. Janz

Molten Salts: Volume 5, Part 1. Additional Single and Multi-Component Salt Systems - Electrical Conductance, Density, Viscosity, and Surface Tension Data
G. J. Janz and R. P. T. Tomkins

Pair, Triplet, and Total Atomic Cross Sections (and Mass Attenuation Coefficients) for 1 MeV-100 GeV Photons in Elements Z=1 to 100
J. H. Hubbell, H. A. Gimm, and I. Øverbø

Tables of Molecular Vibrational Frequencies, Part 10
T. Shimanouchi, H. Matsuura, Y. Ogawa, and I. Harada

An Improved Representative Equation for the Dynamic Viscosity of Water Substance
J. T. R. Watson, R. S. Basu, and J. V. Sengers

Static Dielectric Constant of Water and Steam
M. Uematsu and E. U. Franck

Compilation and Evaluation of Solubility Data in the Mercury (I) Chloride - Water System
Y. Marcus

NSRDS-NBS Series

Selected Tables of Atomic Spectra, Atomic Energy Levels and Multiplet Tables, O V
C. E. Moore
NSRDS-NBS 3, Section 9

EPA/NIH Mass Spectral Data Base, Supplement I and Cumulative Index
S. R. Heller and G. W. A. Milne
NSRDS-NBS 63 Supplement

Ion Energetics Measurements, Supplement I. 1971-1973.
H. M. Rosenstock, D. Sims, S. S. Schroyer, and W. J. Webb
NSRDS-NBS 66

Table of Recommended Rate Constants for Chemical Reactions Occurring in Combustion
Francis Westley
NSRDS-NBS 67

Tables of Line Spectra of the Elements. Part 1. Wavelengths and Intensities. Part 2. Transition Probabilities
J. Reader, C. H. Corliss, W. L. Wiese, and G. A. Martin
NSRDS-NBS 68

Data Publications from Other Publishers

Chemical Kinetic and Photochemical Data Sheets for Atmospheric Reactions
R. F. Hampson
U.S. Department of Transportation, Federal Aviation Administration
FAA-EE-80-17

LNG Materials & Fluids, A User's Manual of Property Data in Graphic Format, Second Supplement
Douglas Mann, Editor
Cryogenics Division, NBS, Boulder, CO

Data Publications in Other NBS Series

Physical Properties Data for Rock Salt
L. H. Gevantman, Editor
NBS Monograph 167

Selected Values of Chemical Thermodynamic Properties: Compounds of Uranium, Protactinium, Thorium, Actinium, and the Alkali Metals
D. D. Wagman, W. H. Evans, V. B. Parker, R. H. Schumm, and R. L. Nuttall
NBS Technical Note 270-8

The Thermochemical Properties of Uranium-Halogen Containing Compounds
V. B. Parker
NBSIR 80-2029

Bibliographies and Indexes in NBS Series

Bibliography on Atomic Transition Probabilities (November 1977 through March 1980)
B. J. Miller, J. R. Fuhr, and G. A. Martin
NBS Spec. Publ. 505-1

Bibliography of Low Energy Electron and Photon Cross Section Data (1978)
J. W. Gallagher and E. C. Beatty
JILA Information Center Report No. 18

Bibliography on Atomic Energy Levels and Spectra, July 1975 through June 1980
R. Zalubas and A. A. Albright
NBS Spec. Publ. 363, Supplement 2

Summary of On-Line or Interactive Physico-Chemical Numerical Data Systems
J. Hilsenrath
NBS Technical Note 1122

Bibliographies and Indexes from Other Publishers

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Volume 12, 1979
Radiation Chemistry Data Center
Radiation Laboratory
University of Notre Dame
Notre Dame, IN 46556

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Volume 13, 1980
Radiation Chemistry Data Center
Radiation Laboratory
University of Notre Dame
Notre Dame, IN 46556

Bulletin of Chemical Thermodynamics, Volume 23, 1980
IUPAC Commission on Thermodynamics and Thermochemistry
Robert D. Freeman, Editor

Data Handling for Science and Technology, An Overview and Sourcebook
S. A. Rossmassler and D. G. Watson
North-Holland Publishing Co., Amsterdam and New York

Miscellaneous Publications by OSRD Staff

The Charge Distribution of ^{12}C
L. S. Cardman, J. W. Lightbody, Jr., S. Penner, S. P. Fivozinsky, X. K. Maruyama, W. P. Trower, and S. E. Williamson
Physics Letters 91B, 203 (1980)

A Computer Based File of X-ray and Electron Beam Central Axis Depth Dose Data for Use in Radiotherapy
J. A. Purdy, W. B. Harms, and S. P. Fivozinsky
Proceedings of the Symposium on Computer Applications in Medical Care, IEEE (1980)

Special Features of NBS's Omnidata System Applicable to the Retrieval, Analysis, and Dissemination of Chemical Data
Bettijoyce B. Molino
Journal of Chemical Information and Computers Sciences, Volume 20 (1980)

Investigations of the Assumptions of the Multiple-Scattering Method for Electron-Molecule Scattering Cross-sections
J. R. Rumble, Jr. and D. G. Truhlar
J. Chem. Phys. 72, 3206 (1980)

Comparison of Local Exchange Potentials for Electron-N_2 Scattering
J. R. Rumble, Jr. and D. G. Truhlar
J. CHem. Phys. 72, 5223 (1980)

CIAMDA - An Index to the Literature on Atomic and Molecular Collision Data Relevant to Fusion Research
J. Rumble, Jr. et al., Eds.
International Atomic Energy Agency, Vienna, Austria (1980)

International Bulletin on Atomic and Molecular Data for Fusion
K. Katsonis and J. Rumble, Jr., Eds.
Issued quarterly by International Atomic Energy Agency, Vienna, Austria (1980)

Publications Scheduled for 1981

Journal of Physical and Chemical Reference Data, Volume 10

Evaluated Kinetic Data for High Temperature Reactions. Volume 4. Homogeneous Gas-Phase Reactions of Halogen Cyanide-Containing Species
D. L. Baulch, J. Duxbury, S. J. Grant, and D. C. Montague

Activity and Osmotic Coefficients of Aqueous Alkali Metal Nitrites
Bert R. Staples

Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. I. Selenium
U. Gaur, H. C. Shu, A. Metita, and B. Wunderlich

Heat Capacity and Other Thermodynamic Properties of Linear Macromolecules. II. Polyethylene
U. Gaur and B. Wunderlich

Atomic Transition Probabilities for Iron, Cobalt, and Nickel (A Critical Data Compilation of Allowed Lines)
J. R. Fuhr, G. A. Martin, W. L. Wiese, and S. M. Younger

Evaluated Activity and Osmotic Coefficients for Aqueous Solutions: Bi-Univalent Compounds of Zinc, Cadmium, and Ethylene bis (trimethylammonium) Chloride and Iodide
Robert N. Goldberg

Ion Product of Water Substance, 0-1000 °C, 1-10,000 bar
W. L. Marshall and E. U. Franck

Tables of the Dynamic and Kinematic Viscosity of Aqueous KCl Solutions in the Temperature Range 25-150 °C and the Pressure Range 0.1-35 MPa
J. Kestin and H. Khalifa, and R. J. Correia

Tables of the Dynamic and Kinematic Viscosity of Aqueous NaCl Solutions in the Temperature Range 20-150 °C and the Pressure Range 0.1-35 MPa
J. Kestin and H. Khalifa

NSRDS-NBS Series

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

Physical Property Data Compilations Relevant to Energy Storage, IV. Flywheels: Data on Metals and Metal Alloys
H. M. Ledbetter
NSRDS-NBS 61, Part IV

Optical Spectra of Nonmetallic Inorganic Transients in Aqueous Solutions
Gordon L. Hug
NSRDS-NBS

Physical Properties Data Compilations Relevant to Energy Storage, Part VI. Molten Salts Project III - Phase C
George J. Janz
NSRDS-NBS

Bibliographies and Indexes in NBS Series

Publications of the National Standard Reference Data System with Author, Materials, and Property Indexes
G. Sherwood

A Catalog of Data Compilations on Photochemical and Photophysical Processes in Solution
J. G. Brummer, W. P. Helman, and A. B. Ross
NBS Spec. Publ. 578

Data Index for Energy Transfer Collisions of Atoms and Molecules, 1970-1979
J. Van Blerkon, J. W. Gallagher, E. C. Beaty, and J. R. Rumble, Jr.
NBS Spec. Publ. 593

Bibliographies and Indexes from Other Publishers

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Volume 13, 1980
Radiation Chemistry Data Center

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Volume 14, 1981
Radiation Chemistry Data Center

Bulletin of Chemical Thermodynamics, Volume 24 (1981)
IUPAC Commission on Thermodynamics and Thermochemistry
Robert D. Freeman, Editor

Equilibrium Properties of Fluid Mixtures, A Bibliography of Data on Fluids of Cryogenic Interest, Second Edition
M. J. Hiza, A. J. Kidnay, and R. C. Miller

Invited Talks and Presentations by OSRD Staff

Activities of the National Standard Reference Data System, ASEE Annual Meeting, University of Massachusetts, Amherst, Massachusetts, June 23, 1980
Sherman P. Fivozinsky

A Review of Central Axis Depth Dose Data for Linear Accelerators, AAPM Annual Meeting, Minneapolis, Minnesota, July 30, 1980
Sherman P. Fivozinsky

Comments on the Role of Engineering Judgment and the Computer in the Management of Material Property Data, ASME Annual Meeting, San Francisco, California, August 14, 1980
Sherman P. Fivozinsky

Compilation and Evaluation of Radiation Depth Dose Data from Electron Accelerators Used for Radiotherapy: Experiences of a Pilot Data Project in a Hospital Environment, Seventh International CODATA Conference, Kyoto, Japan, October 9, 1980
Sherman P. Fivozinsky

Presentation on OSRD to the First Workshop on the DOE/STOR Technical Management Information Systems; also chaired a committee on the need for data in energy storage, Callaway Gardens, Georgia, December 1979
Lewis H. Gevantman

Progress Report on OSRD to the Radiation Chemistry Data Center Advisory Board, University of Notre Dame, Indiana, April 1980
Lewis H. Gevantman

Presentation on Office of Standard Reference Data to the EPA Modeling Group, April 1980
Lewis H. Gevantman

Presentation before the Numerical Data Advisory Board, NAS/NRC, on the project at Lawrence Livermore Laboratory, July 1980
Lewis H. Gevantman

The Office of Standard Reference Data's Role in Disseminating Critically Evaluated Data - presented to 30 librarians at Catholic University seminar
Cynthia A. Goldman

Gordon Conference: Scientific Information Problems in Research, Panel Discussion Summarizing Results in Conference, Plymouth, New Hampshire, July 1980
David R. Lide, Jr.

Critical Evaluation of Data and National and International Data Programs, UNESCO-CODATA Training Course in Data Dissemination, Tsukuba, Japan, October 1980
David R. Lide, Jr.

Reference Data Activities in the United States, University of Tokyo, Tokyo, Japan, October 1980
David R. Lide, Jr.

Omnidata and Related Software as Developed and Applied by the Office of Standard Reference Data for On-Line Retrieval, Analysis, and Manipulation of NSRDS Data Bases, Seventh International CODATA Conference, Kyoto, Japan
Bettijoyce B. Molino

Seminar on Electron Scattering by N_2 - Models that Work, Max Planck Institute, Gottingen, West Germany, February 1980
John R. Rumble, Jr.

The National Bureau of Standards and the National Standard Reference Data System, American Institute of Chemical Engineers (AIChE), 88th National Meeting, Philadelphia Civic Center, Philadelphia, Pennsylvania, June 1980
Howard J. White, Jr.

Technical and Professional Committee Participation and Leadership

David R. Lide, Jr.

Overseer's Visiting Committee, Department of Chemistry, Harvard University

Council of the American Physical Society (APS)

Committee on Congressional Fellows, APS

Committee on Fellowships, Division of Chemical Physics, APS

Committee on Meetings, APS

1981 Irving Langmuir Prize Committee, APS

American Institute of Physics (AIP) Publication Board (Chairman)

Subcommittee on an Anniversary Physics Handbook (Chairman), AIP's 50th Anniversary Celebration Committee

Committee on Nomenclature, ACS

Division of Physical Chemistry, ACS (Alternate Councilor)

Chemical Abstracts Advisory Board, 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 (U.S. Delegate to CODATA & Member of Executive Committee)

CODATA Publication Committee (Chairman)

CODATA Bulletin (Associate Editor)

Program Committee for Seventh International CODATA Conference

Joint Committee on Atomic and Molecular Physical Data (JCAMP)

Interdivisional Committee on Nomenclature and Symbols, IUPAC

Commission on Symbols, Terminology, and Units, IUPAC (Chairman)

Physical Chemistry Division, IUPAC (Vice -President)

Chemical Information System (CIS) Steering Committee (Chairman)

Journal of Physical Chemistry Editorial Search Committee

NAS/NRC Committee on Atomic and Molecular Science

Program Committee, Second International Conference on Precision Measurement and Fundamental Constants

Lewis H. Gevantman

IUPAC Commission V.8 on Solubility Data (CoSecretary)

Source Selection Board, Department of the Army, Medical Bioengineering Research and Development Laboratory

Executive Committee, Joint Committee on Atomic and Molecular Physical Data

Subcommittee on the Chemical Substance Information Network (CSIN)

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

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

Subcommittee on Batteries of the Advisory Committee on Energy Storage to the Department of Energy

Howard J. White, Jr.

International Association for the Properties of Steam, American Society of Mechanical Engineers (ASME) (Executive Secretary)

Task Group on the Internationalization and Systematization of Thermodynamic Tables, Committee on Data for Science and Technology (CODATA/ICSU) (Chairman)

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

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

Project Aspen, MIT (Advisory Committee Member)

Coal Conversion Systems Technical Data Book, Institute of Gas Technology (Advisory Committee Member)

Design Institute for Physical Properties Data, American Institute of Chemical Engineers (Liaison Committee Member)

American Petroleum Institute

Sherman P. Fivozinsky

AAPM Medical Physics Data Group

NBS Nuclear Waste Study Group

Bettijoyce B. Molino

Advisory Group for NBS Computer Configurations

Technical Evaluation Subcommittee for a Univac Proposal

Alice A. Dugan

NML Administrative Council

NML-EEO Women's Personnel Panel, NBS

NBS Seminars Sponsored by OSRD

January 16, 1980

The DOE/STOR Technical Management Information System
Viktor Hampel, Lawrence Livermore Laboratory, Livermore, CA

March 6, 1980

Search and Retrieval of Chemical Compounds through the DARC System (A molecular connectivity search system developed in France)
David G. Watson, Cambridge Crystallographic Data Centre, Cambridge, England

April 17, 1980

The National Nuclear Data Center
Sol Pearlstein, Brookhaven National Laboratory, Upton, L.I., NY

May 20, 1980

Trends in Use of On-Line Data Bases and Systems
Martha Williams, University of Illinois, Champaign-Urbana, IL

September 8, 1980

Information Utilization in an Industrial Research Company
Patricia Lorenz, Exxon Research and Engineering Company, Linden, NJ

October 24, 1980

The Atomic and Molecular Data for Fusion Program of the IAEA - Perspectives and Problems
John R. Rumble, Jr., National Bureau of Standards, Gaithersburg, MD

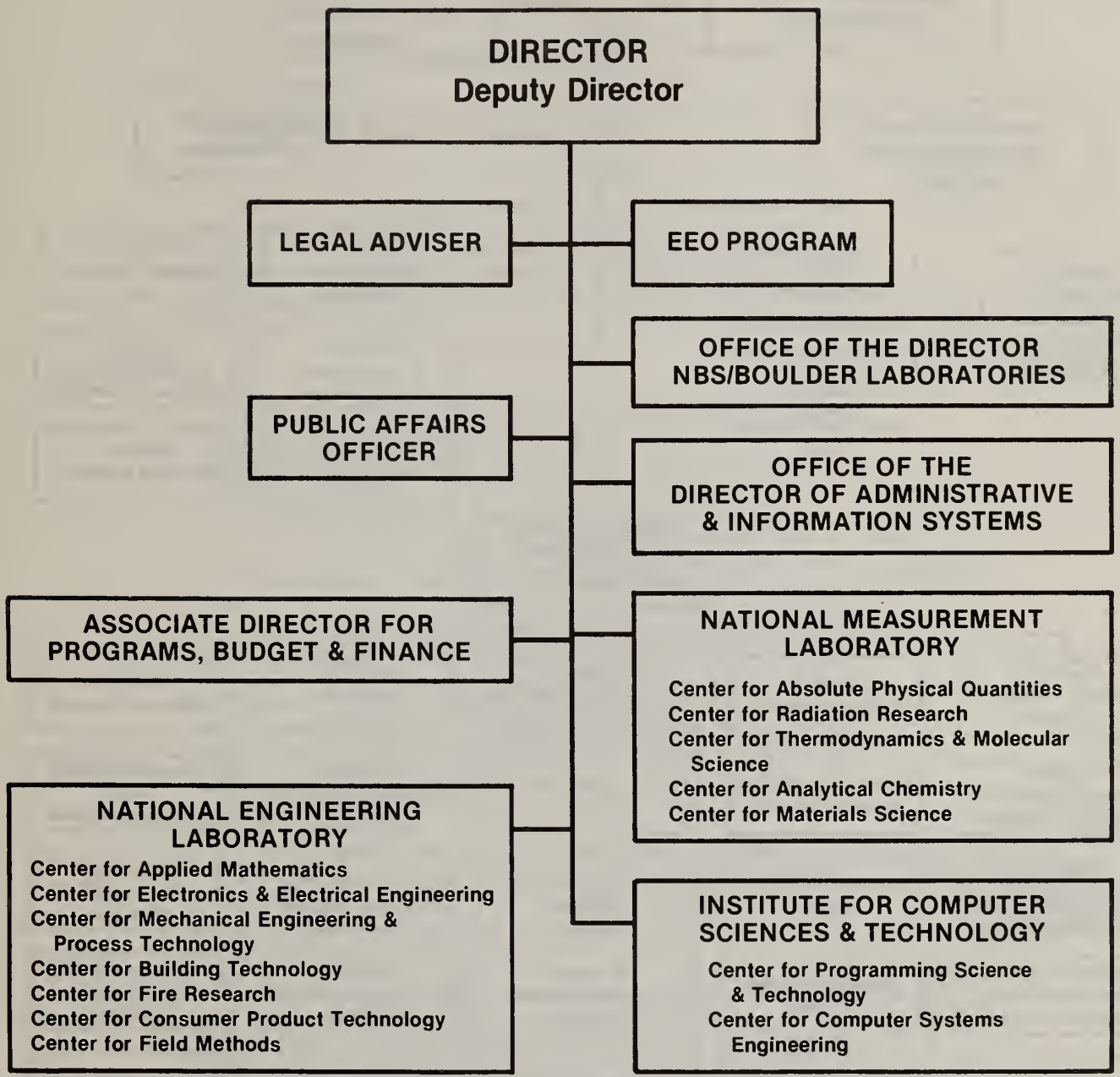
November 3, 1980

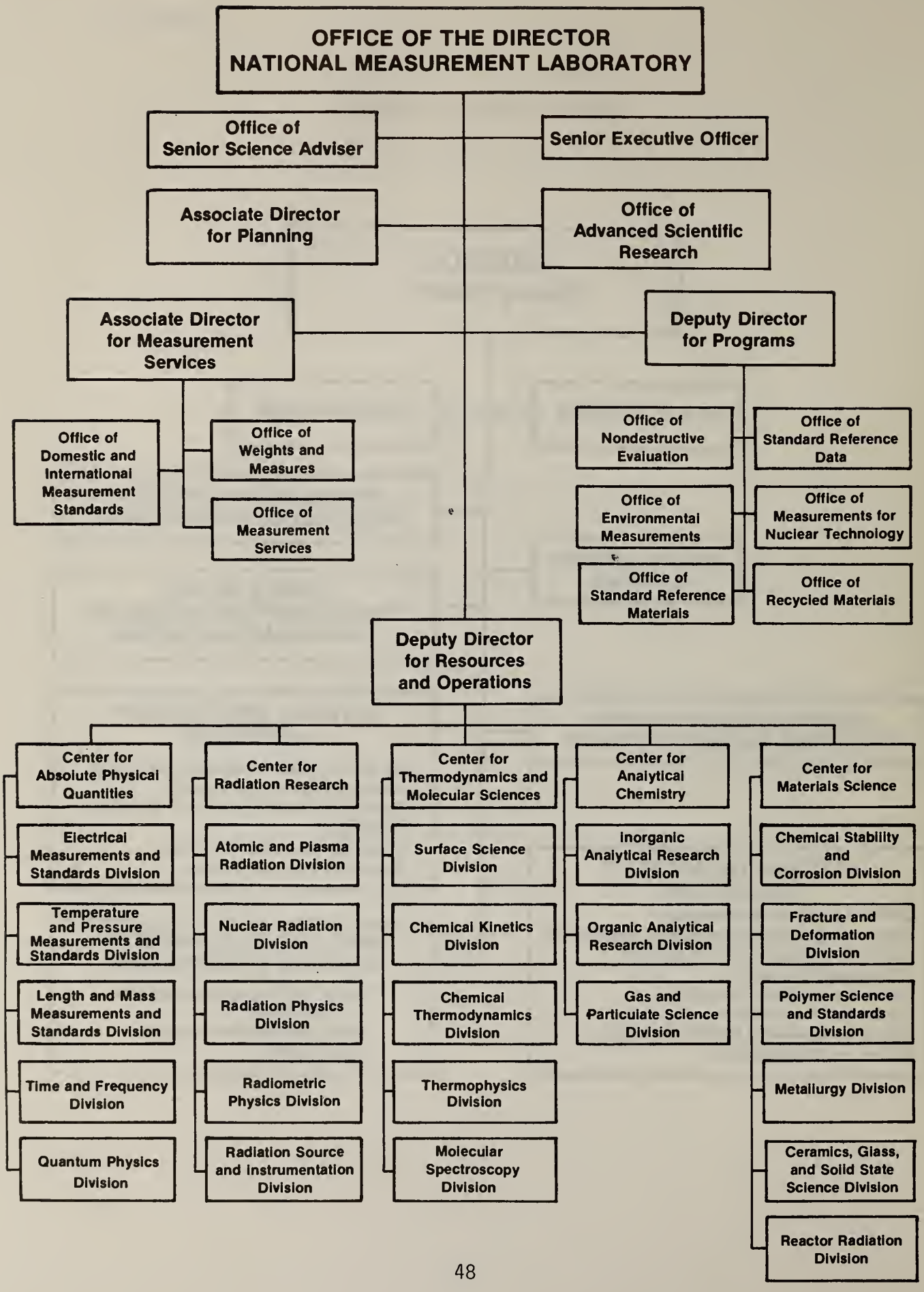
A Computer Based File of X-Ray and Electron Beam Central Axis Depth-Dose Data for Use in Radiation Therapy
James A. Purdy, Washington University School of Medicine, St. Louis, MO

December 10, 1980

The Metal Properties Council Plan for a Computer Data Base of Mechanical Properties
Adolph Schafer, Metal Properties Council, New York, NY

NATIONAL BUREAU OF STANDARDS

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Associate Director for Planning
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Office of Weights and Measures
Office of Measurement Services
Office of Nondestructive Evaluation
Office of Standard Reference Data
Office of Environmental Measurements
Office of Measurements for Nuclear Technology
Office of Standard Reference Materials
Office of Recycled Materials
Deputy Director for Resources and Operations
Center for Absolute Physical Quantities
Electrical Measurements and Standards Division
Temperature and Pressure Measurements and Standards Division
Length and Mass Measurements and Standards Division
Time and Frequency Division
Quantum Physics Division
Center for Radiation Research
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Metallurgy Division
Ceramics, Glass, and Solid State Science Division
Reactor Radiation Division

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).
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Vol. 114 (1968): June 13, considered and passed Senate, amended.
June 27, House concurred in Senate amendments.

GPO 98-139

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

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NATIONAL BUREAU OF STANDARDS
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WASHINGTON, D.C. 20234

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10. SUPPLEMENTARY NOTES

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

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

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

The Office of Standard Reference Data is responsible for management and coordination of the program. Work is carried out through a decentralized network of data centers and projects referred to as the National Standard Reference Data System (NSRDS). This volume summarizes the activities of the Program for the year 1980.

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

data compilation; energy and environmental data; evaluated data; materials data; standard reference data; thermochemical and thermophysical data; technical activities 1980

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