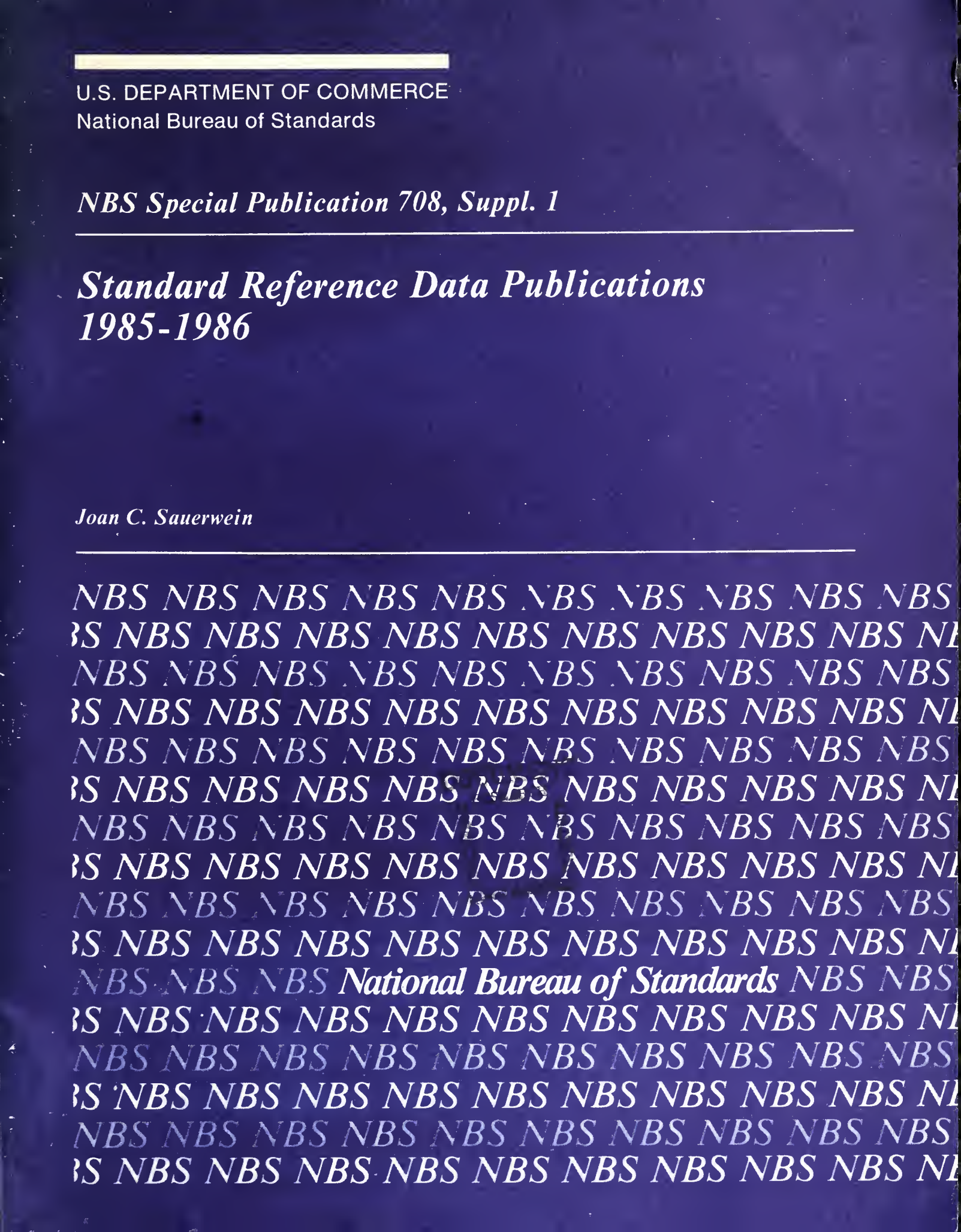
U.S. DEPARTMENT OF COMMERCE
National Bureau of Standards

NBS Special Publication 708, Suppl. 1

Standard Reference Data Publications 1985-1986

Joan C. Sauerwein



The National Bureau of Standards[1] was established by an act of Congress on March 3, 1901. The Bureau's overall goal is to strengthen and advance the nation's science and technology and facilitate their effective application for public benefit. To this end, the Bureau conducts research to assure international competitiveness and leadership of U.S. industry, science and technology. NBS work involves development and transfer of measurements, standards and related science and technology, in support of continually improving U.S. productivity, product quality and reliability, innovation and underlying science and engineering. The Bureau's technical work is performed by the National Measurement Laboratory, the National Engineering Laboratory, the Institute for Computer Sciences and Technology, and the Institute for Materials Science and Engineering.

The National Measurement Laboratory

Provides the national system of physical and chemical measurement; coordinates the system with measurement systems of other nations and furnishes essential services leading to accurate and uniform physical and chemical measurement throughout the Nation's scientific community, industry, and commerce; provides advisory and research services to other Government agencies; conducts physical and chemical research; develops, produces, and distributes Standard Reference Materials; provides calibration services; and manages the National Standard Reference Data System. The Laboratory consists of the following centers:

- Basic Standards[2]
- Radiation Research
- Chemical Physics
- Analytical Chemistry

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- Applied Mathematics
- Electronics and Electrical Engineering[2]
- Manufacturing Engineering
- Building Technology
- Fire Research
- Chemical Engineering[3]

The Institute for Computer Sciences and Technology

Conducts research and provides scientific and technical services to aid Federal agencies in the selection, acquisition, application, and use of computer technology to improve effectiveness and economy in Government operations in accordance with Public Law 89-306 (40 U.S.C. 759), relevant Executive Orders, and other directives; carries out this mission by managing the Federal Information Processing Standards Program, developing Federal ADP standards guidelines, and managing Federal participation in ADP voluntary standardization activities; provides scientific and technological advisory services and assistance to Federal agencies; and provides the technical foundation for computer-related policies of the Federal Government. The Institute consists of the following divisions:

- Information Systems Engineering
- Systems and Software Technology
- Computer Security
- Systems and Network Architecture
- Advanced Computer Systems

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Conducts research and provides measurements, data, standards, reference materials, quantitative understanding and other technical information fundamental to the processing, structure, properties and performance of materials; addresses the scientific basis for new advanced materials technologies; plans research around cross-cutting scientific themes such as nondestructive evaluation and phase diagram development; oversees Bureau-wide technical programs in nuclear reactor radiation research and nondestructive evaluation; and broadly disseminates generic technical information resulting from its programs. The Institute consists of the following Divisions:

- Ceramics
- Fracture and Deformation[3]
- Polymers
- Metallurgy
- Reactor Radiation

[1]Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Gaithersburg, MD 20899.
[2]Some divisions within the center are located at Boulder, CO 80303.
[3]Located at Boulder, CO, with some elements at Gaithersburg, MD

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Office of Standard Reference Data
National Bureau of Standards
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U.S. Department of Commerce
Malcolm Baldrige, Secretary

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Foreword

The National Standard Reference Data System was established in 1963 for the purpose of promoting the critical evaluation and dissemination of numerical data of the physical sciences. The program is coordinated by the Office of Standard Reference Data of the National Bureau of Standards but involves the efforts of many groups in universities, government laboratories, and private industry. The primary aim of the program is to provide compilations of critically evaluated physical and chemical property data. These tables are published in the Journal of Physical and Chemical Reference Data, in the NSRDS-NBS series of the National Bureau of Standards, and through other appropriate channels. Other outputs of the program include bibliographies, computer programs for handling data, and databases in magnetic tape and disk formats.

This listing includes all publications which have appeared in the period 1985–86. It supplements "Standard Reference Data Publications 1964–1984", NBS SP 708. Indexes to authors, properties, and material classes are given, as well as information on ordering publications.

David R. Lide, Director
Office of Standard Reference Data

Contents

Standard Reference Data Publications 1985–1986

Joan C. Sauerwein

Office of Standard Reference Data, National Bureau of Standards, Gaithersburg, MD 20899

The National Bureau of Standards' Office of Standard Reference Data manages a network of data centers that prepare evaluated databases of physical and chemical properties of substances. Databases are available in printed form, on magnetic tapes, diskettes, and through on-line computer networks. This document provides a comprehensive list of the products available from the National Standard Reference Data System (NSRDS) for the years 1985–1986, including indexes qualified by author, material, and property terms. Ordering information and current prices can be found at the end of this document.

Key words: bibliographies; chemical properties; evaluated data; indexes; materials properties; physical properties; publication list.

Introduction

The National Standard Reference Data System (NSRDS), established in 1963, coordinates on a national scale the compilation and dissemination of reference data in the physical sciences. Under the Standard Reference Data Act (Public Law 90–396) the National Bureau of Standards (NBS) of the U.S. Department of Commerce has the primary responsibility in the Federal Government for providing reliable scientific and technical data. The Office of Standard Reference Data at NBS coordinates a complex of data evaluation centers, located in university, industrial, and other Government laboratories as well as within NBS. These centers compile and critically evaluate numerical physical and chemical property data retrieved from the world's scientific literature.

This publications list includes NSRDS data compilations, critical reviews, and other publications which are available from various sources. Indexes by author, property, and materials class are included. Prices and ordering instructions for publications listed are given in this document and further information may be obtained from:

Office of Standard Reference Data
National Bureau of Standards
Gaithersburg, MD 20899

Reprints

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Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C_1 to C_4. Part 1. Properties of Condensed Phases—Randolph C. Wilhoit, Jing Chao, and Kenneth R. Hall. J. Phys. Chem. Ref. Data **14**, 1 (1985).

A survey of the published values of heat capacity and enthalpy obtained from calorimetric measurements on the crystal, glass and liquid phases of the first few members of homologous series of organic oxygen compounds is presented. Equations for the heat capacities expressed as polynomial functions of temperature were fit to selected data by a least squares procedure. Tables of smoothed values of thermodynamic properties, derived from these functions, are presented for 38 compounds.

266

Standard Chemical Thermodynamic Properties of Alkylbenzene Isomer Groups—Robert A. Alberty. J. Phys. Chem. Ref. Data **14**, 177 (1985).

The chemical thermodynamic properties of alkylbenzene isomer groups from C_8H_{10} to C_9H_{12} in the ideal gas phase have been calculated from 298.15 to 1000 K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers of $C_{10}H_{14}$ to $C_{12}H_{18}$ have been calculated using Benson group values. For isomer group properties, increments per carbon atom have been calculated to show the extent to which thermodynamic properties of higher isomer groups may be obtained by linear extrapolation.

267

Asessment of Critical Parameter Values for H_2O and D_2O—J. M. H. Levelt Sengers, J. Straub, K. Watanabe, and P. G. Hill. J. Phys. Chem. Ref. Data **14**, 193 (1985).

Recommendations for the most likely values of the critical parameters of light and heavy water as accepted by the International Association for the Properties of Steam are presented, together with an assessment of their reliability. Supporting material for these choices of values and the assessment of their reliability is provided. Temperature values are on the International Practical Temperature Scale of 1968 (IPTS 1968) unless otherwise indicated.

268

The Viscosity of Nitrogen, Oxygen, and Their Binary Mixtures in the Limit of Zero Density—Wendy A. Cole and William A. Wakeham. J. Phys. Chem. Ref. Data **14**, 209 (1985).

The paper presents a concise and accurate representation of the viscosity of nitrogen, oxygen, and their binary mixtures at the limit of zero density and in the temperature range 110–2100 K, which can be programmed easily on a computer. The correlation is founded upon the semiclassical kinetic theory of polyatomic gases and a body of critically evaluated experimental data. Use is also made of the principle of corresponding states to extend the correlation outside of the temperature range for which experimental results exist.

269

The Thermal Conductivity of Fluid Air—K. Stephan and A. Laesecke. J. Phys. Chem. Ref. Data **14**, 227 (1985).

Based on available experimental data, the thermal conductivity of fluid air has been critically evaluated. A new set of recommended values is presented covering a pressure range from 1 to 1000 bar and a temperature range from 70 to 1000 K. Using the concept of residual thermal conductivity, the recommended values are described by a 13-parameter equation of state in terms of temperature and density which may be applied to a density of 900 kg/m^3. From comparisons of all data sources, the uncertainty of the recommended values was estimated to be below ±4% Additional experiments are needed, especially in the subcritical region of liquid air.

270

The Electronic Spectrum and Energy Levels of the Deuterium Molecule—Robert S. Freund, James A. Schiavone, and H. M. Crosswhite. J. Phys. Chem. Ref. Data **14**, 235 (1985).

This paper gives the 27,488 lines of molecular deuterium, measured by G. H. Dieke, arranges the 8243 assigned lines into band systems, and derives rotational-vibrational energy levels for over 50 electronic states. It also derives energy levels from the published vacuum ultraviolet spectra of D_2.

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Microwave Spectra of Molecules of Astrophysical Interest. XXII. Sulfur Dioxide (SO_2)—F. J. Lovas. J. Phys. Chem. Ref. Data **14**, 395 (1985).

The microwave spectrum of sulfur dioxide (SO_2) is critically reviewed and supplemented with spectral frequency calculations derived from rotational and centrifugal distortion terms in the molecular Hamiltonian. Microwave transition frequencies applicable to molecular radio astronomy for the ground vibrational state of the most abundant isotopic forms are provided.

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Evaluation of the Thermodynamic Functions for Aqueous Sodium Chloride from Equilibrium and Calorimetric Measurements below 154 °C—E. Colin W. Clarke and David N. Glew. J. Phys. Chem. Ref. Data **14**, 489 (1985).

A new weighted least-squares method is described which is generally applicable for the nonsubjective evaluation of the best set of thermodynamic functions from a given data set of equilibrium (ΔG) and calorimetric ($\Delta H, C_p$) measurements. The method, applied to model a wide range of 2428 measurements of the water-sodium chloride system between −21 and 154 °C, accurately represents all measurements within experimental error. The resulting model is used to predict the thermodynamic functions and their standard errors for aqueous sodium chloride up to 110 °C.

273

The Mark-Houwink-Sakurada Equation for the Viscosity of Linear Polyethylene—Herman L. Wagner. J. Phys. Chem. Ref. Data **14**, 611 (1985).

In this review, the parameters K and α found in the literature for the Mark-Houwink-Sakurada equation relating viscosity to molecular weight have been critically evaluated for linear polyethylene, and values have been recommended for six commonly used solvents. These are decalin, 1,2,4- tricholorobenzene, 1-chloronaphthalene, tetralin, *o*- dichlorobenzene, and *p*-xylene.

274

The Solubility of Mercury and Some Sparingly Soluble Mercury Salts in Water and Aqueous Electrolyte Solutions—H. Lawrence Clever, Susan A. Johnson, and M. Elizabeth Derrick. J. Phys. Chem. Ref. Data **14**, 631 (1985).

The literature on the solubility of mercury and of the sparingly soluble salts of mercury (I) and mercury (II) in water and in aqueous electrolyte solutions has been reviewed. The solubility data have been compiled and evaluated. Recommended and tentative values of the solubilities are presented when warranted. Auxiliary thermodynamic data and crystallographic data useful in the interpretation of solubility of some of the less common inorganic mercury compounds, with emphasis on the sol[illegible] since 1950, is given.

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A Review and Evaluation of the Phase Equilibria, Liquid-Phase Heats of Mixing and Excess Volumes, and Gas-Phase *PVT* Measurements for Nitrogen + Methane—A. J. Kidnay, R. C. Miller, E. D. Sloan, and M. J. Hiza. J. Phys. Chem. Ref. Data **14**, 681 (1985).

The available experimental data for vapor-liquid equilibria, heat of mixing, change in volume on mixing for liquid mixtures, and gas- phase *PVT* measurements for nitrogen + methane have been reviewed and where possible evaluated for consistency. The derived properties chosen for analysis and correlation were liquid mixture excess Gibbs free energies, and Henry's constants.

276

The Homogeneous Nucleation Limits of Liquids—C. T. Avedisian. J. Phys. Chem. Ref. Data **14**, 695 (1985).

This work provides a critical compilation of the homogeneous nucleation limits of liquids. Data for 90 pure substances and 28 mixtures have been compiled over a range of pressures, nucleation rates, and compositions. Detailed descriptions of the experimental methods used to obtain the included data are given to assess the accuracy of measured values. Criteria used to select the measurements included in the final listing are discussed.

277

Binding Energies in Atomic Negative Ions. II—H. Hotop and W. C. Lineberger. J. Phys. Chem. Ref. Data **14**, 731 (1985).

This article updates a ten-year review of this subject [J. Phys. Chem. Ref. Data **4**, 539(1975)]. A survey of the electron affinity determinations for the elements $Z = 85$ is presented, and based upon these data, a set of recommended electron affinities is established. Recent calculations of atomic electron affinities and the major semiempirical methods are discussed and compared with experiment. The experimental methods which yield electron binding energy data are described and intercompared. Fine structure splittings of these ions and excited state term energies are given.

278

Energy Levels of Phosphorous, P I through P XV—W. C. Martin, Romuald Zalubas, and Arlene Musgrove. J. Phys. Chem. Ref. Data **14**, 751 (1985).

Energy level data are given for the atom and all positive ions of phosphorous ($Z = 15$). These data have been critically compiled, mainly from published and unpublished material on measurements and analyses of the optical spectra. The levels for a number of the ions have been derived or recalculated. In addition to the level values in cm^{-1} and the parity, the J value and the configuration and term assignments are listed if known. Leading percentages from the calculated eigenvectors are tabulated or quoted wherever available. Ionization energies are given for all spectra.

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Standard Chemical Thermodynamic Properties of Alkene Isomer Groups—Robert A. Alberty and Catherine A. Gehrig. J. Phys. Chem. Ref. Data **14**, 803 (1985).

The chemical thermodynamic properties of alkene isomer groups from C_4H_8 to C_6H_{12} in the ideal gas phase have been calculated from 298.15 to 1000 K from the tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers C_7H_{14} to C_8H_{16} have been estimated using the Benson group values. Equilibrium mole fractions within isomer groups have been calculated for the ideal state from 298.15 to 1000 K.

280

Standard Chemical Thermodynamic Properties of Alkylnaphthalene Isomer Groups—Robert A. Alberty and Theodore M. Bloomstein. J. Phys. Chem. Ref. Data **14**, 821 (1985).

The chemical thermodynamic properties of alkinaphthalene isomer groups for $C_{10}H_8$ and $C_{11}H_{10}$ in the ideal gas phase have been calculated from 298.15 to 1000 K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers of $C_{12}H_{12}$ to $C_{14}H_{16}$ have been calculated using Benson group values.

281

Carbon Monoxide Thermophysical Properties from 68 to 1000 K at Pressures to 100 MPa—Robert D. Goodwin. J. Phys. Chem. Ref. Data **14**, 849 (1985).

An improved form of the nonanalytical equation of state is used to compute thermodynamic properties of carbon monoxide along isobars up to 100 MPa, at integral temperatures from coexistence to 1000 K.

282

Refractive Index of Water and Its Dependence on Wavelength, Temperature, and Density—I. Thormählen, J. Straub, and U. Grigull. J. Phys. Chem. Ref. Data **14**, 933 (1985).

A survey of the available experimental data and the existing equations for the refractive index of water is given. The dependence of the molar refraction on wavelength, temperature, and density is shown over an extended range. Based on the electromagnetic theory of light an equation for the refractive index of water with wavelength, temperature, and density as independent variables is constructed. Its coefficients are directly deduced from all available experimental data by least-squares fit.

283

Viscosity and Thermal Conductivity of Dry Air in the Gaseous Phase—K. Kadoya, N. Matsunaga, and A. Nagashima. J. Phys. Chem Ref. Data **14**, 947 (1985).

In view of the importance of air in science and technology and the abundance of experimental data, a consistent set of critically evaluated data and an up-to-date correlation of the viscosity and the thermal conductivity of air in the gaseous phase over a wide range of temperature and pressure is presented. This is especially important for the viscosity, since the recent data show systematic differences compared with the old standard value used for many years. The present paper was written in order to document the critical evaluation of the latest data sets and to present a new set of correlations of the viscosity and the thermal conductivity of air.

284

Charge Transfer of Hydrogen Ions and Atoms in Metal Vapors—T. J. Morgan, R. E. Olson, A. S. Schlachter, and J. W. Gallagher. J. Phys. Chem. Ref. Data **14**, 971 (1985).

Cross sections and equilibrium fractions for energetic H^+, H^-, and H^0 in collisions with metal-vapor targets have been compiled and evaluated. Both experimental and theoretical results are reported. Sources of errors are discussed, and recommended values for the data are presented.

285

Reactivity of HO_2/O_2^- Radicals in Aqueous Solution—Benon H. J. Bielski, Diane E. Cabelli, Ravindra L. Arudi and Alberta B. Ross. J. Phys. Chem. Ref. Data **14**, 1041 (1985).

Kinetic data for the superoxide radical ($HO_2 \rightleftharpoons O_2^- + H^+, pK = 4.8$) in aqueous solution have been critically assessed. Rate constants for reactions of O_2^- and HO_2 with more than 300 organic and inorganic ions, molecules and other transient species have been tabulated.

286

The Mark-Houwink-Sakurada Equation for the Viscosity of Atactic Polystyrene—Herman L. Wagner. J. Phys. Chem. Ref. Data **14**, 1101 (1985).

In this review, the viscosity-molecular weight (Mark-Houwink-Sakurada) relationships have been critically evaluated for atactic polystyrene for a variety of solvents often used for viscosity measurements. These are benzene, toluene, 1,2,4- trichlorobenzene, tetrahydrofuran, *o*-dichlorobenzene, 2-butanone, and two theta solvents, cyclohexane and decalin. In addition, the Mark-Houwink-Sakurada parameters for several other solvents, not used as frequently, are provided.

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Standard Chemical Thermodynamic Properties of Alkylcyclopentane Isomer Groups, Alkylcyclohexane Isomer Groups, and Combined Isomer Groups—Robert A. Alberty and Young S. Ha. J. Phys. Chem. Ref. Data **14**, 1107 (1985).

The standard chemical thermodynamic properties of the alkylcyclopentane isomer groups have been calculated through C_9H_{18} in the ideal gas phase from 298.15 to 1000 K, and the properties of the alkylcyclohexane isomer groups which have been calculated through $C_{10}H_{20}$. The properties of individual species for which literature data are not available have been estimated using the Benson method.

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Triplet-Triplet Absorption Spectra of Organic Molecules in Condensed Phases—Ian Carmichael and Gordon L. Hug. J. Phys. Chem. Ref. Data **15**, 1 (1986).

A compilation of spectral parameters associated with triplet-triplet absorption of organic molecules in condensed media is presented. The wavelengths of maximum absorbance and the corresponding extinction coefficients, where known, have been critically evaluated. An introduction to triplet state processes in solution and solids, developing the conceptual background and offering a historical perspective on the detection and measurement of triplet state absorption is provided.

289

Recommended Rest Frequencies for Observed Interstellar Molecular Microwave Transitions - 1985 Revision—F. J. Lovas. J. Phys. Chem. Ref. Data **15**, 251 (1986).

Accurate transition frequencies for the transitions of the molecular species detected in interstellar clouds are presented. These are recommended for reference in future astronomical observations in the radio and microwave regions. The transition frequencies have been selected through critical examination and analysis of the spectroscopic data in the literature. The species identity, quantum number labels, and probable error limits are presented for each transition. Representative line antenna temperatures are also given for a typical source as a convenience to users. References are cited to both the astronomical and laboratory literature.

290

New International Formulations for the Thermodynamic Properties of Light and Heavy Water—J. Kestin and J. V. Sengers. J. Phys. Chem. Ref. Data **15**, 305 (1986).

The General Assembly of the International Association for the Properties of Steam (IAPS), meeting at the 10th International Conference on the Properties of Steam in Moscow in September 1984, adopted new formulations for the thermodynamic properties of fluid H_2O and D_2O. The new formulations have been designated as the *IAPS Formulation 1984 for the Thermodynamic Properties of Ordinary Water Substance for Scientific and General Use* and the *IAPS Formulation 1984 for the Thermodynamic Properties of Heavy Water Substance*. This paper presents and discusses these new formulations.

291

Forbidden Lines in ns^2np^k Ground Configurations and *nsnp* Excited Configurations of Beryllium through Molybdenum Atoms and Ions—Victor Kaufman and Jack Sugar. J. Phys. Chem. Ref. Data **15**, 321 (1986).

Observed and predicted wavelengths of magnetic dipole lines arising within ground configurations of the type ns^2np^k ($n = 2$ and 3, $k = 1$ to 5) are compiled. For $n = 2$ the compilation includes the elements B through Kr, and for $k = 5$ it extends to Mo. For $n = 3$ Al through Mo are included. In addition the $2s2p$ excited configuration of the Be I isoelectric sequence for Be through Kr and $3s3p$ of the Mg sequence for Mg through Mo are included.

292

Thermodynamic Properties of Twenty-One Monocyclic Hydrocarbons—O. V. Dorofeeva, L. V. Gurvich, and V. S. Jorish. J. Phys. Chem. Ref. Data **15**, 437 (1986).

The available structural parameters, fundamental frequencies, and relative energies of different stable conformers, if any, for cyclopropane, cyclopropene, cyclobutane, cyclobutene, 1-3- cyclobutadiene, cyclopentane, cyclopentene, 1-3-cyclopentadiene, cyclohexane, cyclohexene, 1,3-cyclohexadiene, 1,4-cyclohexadiene, cycloheptane, cycloheptene, 1,3-cycloheptadiene, 1,3,5-cycloheptatriene, cyclooctane, cyclooctene, 1,3-cyclooctadiene, 1,5-cyclooctadiene, and 1,3,5,7-cyclooctatetraene were critically evaluated and the recommended values selected.

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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. J. Phys. Chem. Ref. Data **15**, 465 (1986).

The available kinetic data for the homogeneous gas phase reactions of the hydroxyl radical with alkanes have been compiled and critically evaluated. For each reaction, relevant thermodynamic data, a table of measured rate constants, a discussion of the data, and a comprehensive bibliography are presented. Wherever possible, the preferred rate parameters are given with their associated error limits and temperature ranges.

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Thermodynamic Properties of Ethylene from the Freezing Line to 450 K at Pressures to 260 MPa—Majid Jahangiri, Richard T. Jacobsen, Richard B. Stewart, and Robert D. McCarty. J. Phys. Chem. Ref. Data **15**, 593 (1986).

A new fundamental equation explicit in Helmholtz energy for thermodynamic properties of ethylene from the freezing line to 450 K at pressures to 260 MPa is presented. Independent equations for the vapor pressure for the saturated liquid and vapor densities as functions of temperature, and for the ideal gas heat capacity are also included.

295

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. J. Phys. Chem. Ref. Data **15**, 735 (1986).

A new fundamental equation explicit in Helmholtz energy for thermodynamic properties of nitrogen from the freezing line to 2000 K at pressures to 1000 MPa is presented. New independent equations for the vapor pressure and for the saturated liquid and vapor densities as functions of temperature are also included.

296

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. J. Phys. Chem. Ref. Data **15**, 911 (1986).

Relationships between the environmentally relevant physical chemical properties of the polychlorinated biphenyls, namely, aqueous solubility, vapor pressure, Henry's law constant, and octanol-water partition coefficient are discussed. Reported experimental data are tabulated and critically reviewed. Recommended values are given for 42 of the 209 congeners; however, procedures are suggested for estimating the properties of the other congeners.

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Computer Methods Applied to the Assessment of Thermochemical Data. Part I. The Establishment 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. J. Phys. Chem. Ref. Data **15**, 943 (1986).

Computer methods are described for the storage, retrieval, and processing of large amounts of thermochemical data and related textual material. The procedures are illustrated by a critical evaluation of data for $TiCl_4$(g), $TiCl_4$(l), $TiCl_3$(cr), and $TiCl_2$(cr); values for standard enthalpies of formation and entropies at 298.15 K are selected for these species.

298

Thermodynamic Properties of Iron and Silicon—P. D. Desai. J. Phys. Chem. Ref. Data **15**, 967 (1986).

This work reviews and discusses the data on the various thermodynamic properties of iron and silicon available through March 1984. These include heat capacity, enthalpy, enthalpies of transition and melting, vapor pressure, and enthalpy of vaporization. The recommended values for heat capacity, enthalpy, entropy, and Gibbs energy function cover the temperature range from 1 to 3200 K for iron and 1 to 3600 K for silicon. The recommended values for vapor pressure cover the temperature range from 298.15 to 3200 K for iron and from 298.15 to 3600 K for silicon.

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Cross Sections for Collisions of Electrons and Photons with Nitrogen Molecules—Y. Itikawa, M. Hayashi, A. Ichimura, K. Onda, K. Sakimoto, K. Takayanagi, M. Nakamura, H. Nishimura, and T. Takayanagi. J. Phys. Chem. Ref. Data **15**, 985 (1986).

Data have been compiled on the cross sections for collisions of electrons and photons with nitrogen molecules (N_2). For electron collisions, the processes considered are: total scattering, elastic scattering, momentum transfer, excitations of rotational, vibrational and electronic states, dissociation and ionization. Ionization and dissociation processes are discussed for photon impact. Cross section data selected are presented graphically. Spectroscopic and other properties of the nitrogen molecule are summarized.

300

Thermochemical Data on Gas-Phase Ion-Molecule Association and Clustering Reactions—R. G. Keesee and A. W. Castleman, Jr.. J. Phys. Chem. Ref. Data **15**, 1011 (1986).

A comprehensive tabulation of the standard enthalpy change, $\Delta H°$ entropy change, $\Delta S°$, and free energy change, $\Delta G°$, for the formation of ion clusters from ion-molecule association reactions is given. The experimental methods which are used to derive the data are briefly discussed. For some experiments, dissociation energies of ion clusters are reported and listed under the category of $\Delta H°$. The relationship between $\Delta H°$ and dissociation energy is discussed in the text.

301

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. J. Phys. Chem. Ref. Data **15**, 1073 (1986).

The available experimental liquid-phase thermal conductivity data for water, toluene, and *n*-heptane have been examined with the intention of establishing standard reference values along the saturation line. The quality of available data is such that for toluene and water new standard reference values can be proposed with confidence limits better than ± 1.0% for most of the liquid range. For *n*-heptane there are insufficient reliable experimental data for the system to be treated as a primary reference standard, so a lower quality correlation has been developed which yields a set of secondary reference data with confidence limits of ± 1.5% for most of the normal liquid range.

302

Chemical Kinetic Data Base for Combustion Chemistry. Part I. Methane and Related Compounds—W. Tsang and R. F. Hampson. J. Phys. Chem. Ref. Data **15**, 1087 (1986).

This document contains evaluated data on the kinetics and thermodynamic properties of species that are of importance in methane pyrolysis and combustion. Specifically, the substances considered include H, H_2, O, O_2, OH, HO_2, H_2O_2, H_2O, CH_4, C_2H_6, HCHO, CO_2, CO, HCO, CH_3, C_2H_5, C_2H_4, C_2H_3, C_2H_2, C_2H, CH_3CO, CH_3O_2, CH_3O, singlet CH_2 and triplet CH_2. All possible reactions are considered.

303

Improved International Formulations for the Viscosity and Thermal Conductivity of Water Substance—J. V. Sengers and J. T. R. Watson. J. Phys. Chem. Ref. Data **15**, 1291 (1986).

This paper describes improved international formulations for the viscosity and thermal conductivity of water substance recently adopted by the International Association for the Properties of Steam.

304

The Viscosity and Thermal Conductivity of Normal Hydrogen in the Limit of Zero Density—M. J. Assael, S. Mixafendi, and W. A. Wakeham. J. Phys. Chem. Ref. Data **15**, 1315 (1986).

This paper contains a new representation of the viscosity and thermal conductivity coefficients of normal hydrogen in the limit of zero density as a function of temperature. The correlation is based upon the semiclassical kinetic theory of polyatomic gases and a body of critically evaluated experimental data.

305

The Viscosity and Thermal Conductivity Coefficients of Gaseous and Liquid Argon—B. A. Younglove and H. J. M. Hanley. J. Phys. Chem. Ref. Data **15**, 1323 (1986).

Data for the viscosity and thermal conductivity of gaseous and liquid argon have been evaluated and represented by empirical functions. Tables for the viscosity from 86 to 500 K for pressures to 400 MPa, and for the thermal conductivity from 90 to 500 K for pressures to 200 MPa are presented.

306

Standard Chemical Thermodynamic Properties of Alkyne Isomer Groups—Robert A. Alberty and Ellen Burmenko. J. Phys. Chem. Ref. Data **15**, 1339 (1986).

The chemical thermodynamic properties of alkyne isomer groups from C_2H_2 to C_5H_8 in the ideal gas phase have been calculated from 298.15 to 1000 K from tables of Stull, Westrum, and Sinke. In the absence of literature data on all isomers of higher isomer groups, the properties of isomers of C_6H_{10} to C_8H_{14} have been estimated using Benson group values.

307

Recent Progress in Deuterium Triple-Point Measurements—L. A. Schwalbe. J. Phys. Chem. Ref. Data **15**, 1351 (1986).

The triple point of deuterium is a proposed reference for defining the temperature scale between 13.81 and 24.562 K. Recent measurements of this fixed point are reviewed; the discussion concentrates on experiments with samples confined in transportable sealed cells. Theoretical estimates of the dependence of the triple-point temperature on the spin composition of the sample are also presented.

308

Rate Constants for Reactions of Radiation-Produced Transients in Aqueous Solutions of Actinides—S. Gordon, J. C. Sullivan, and Alberta B. Ross. J. Phys. Chem. Ref. Data 15, 1357 (1986). Rate constants have been critically compiled for reactions of ions of the actinides Am, Cf, Cm, Np, Pu, Th, and U, as well as the element Tc, in different oxidation states with various chemical species in aqueous solution. The reactants include products of the radiolysis of water (hydrated electrons, hydrogen atoms, hydroxyl radicals, hydrogen peroxide) and transient species derived from other solutes (e.g. carbonate radical). The data are useful in the estimation of migration properties of actinides, which are relevant to waste management studies.

309

Thermodynamic Properties of Key Organic Oxygen Compounds in the Carbon Range C_1 to C_4. Part 2. Ideal Gas Properties—Jing Chao, Kenneth R. Hall, Kenneth N. Marsh, and Randolph C. Wilhoit. J. Phys. Chem. Ref. Data 15, 1369 (1986).

The ideal gas thermodynamic properties of forty-four key organic oxygen compounds in the carbon range C_1 to C_4 have been calculated by a statistical mechanical technique. The properties determined are the heat capacity, entropy, enthalpy, and Gibbs energy function. The calculations have been performed, in most cases, over the temperature range 0 to 1500 K and at 1 bar. The contributions to the thermodynamic properties of compounds having internal- or pseudo- rotations have been computed by employing a partition function formed by the summation of the internal rotational or pseudorotational energy levels for each rotor in the given molecule.

Supplements

Supplement 1

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. J. Phys. Chem. Ref. Data 14, Suppl. 1 (1985).

Recommended temperature-dependent values are provided for chemical thermodynamic properties of inorganic substances and for organic substances containing only one or two carbon atoms. These tables cover the thermodynamic properties over a wide range of temperature with single-phase and multiphase tables for the crystal, liquid, and ideal gas state.

Supplement 2

Atomic Energy Levels of the Iron Period Elements: Potassium through Nickel—Jack Sugar and Charles Corliss. J. Phys. Chem. Ref. Data 14, Suppl. 2 (1985).

Experimentally derived energy levels of the elements from potassium to nickel in all stages of ionization are critically compiled. The data for each level include its position in cm^{-1} (relative to the ground state), configuration, term designation, J-value and, where available, the g-value and two leading percentages of the eigenvector composition in the most appropriate coupling scheme. For the He I and the H I isoelectronic sequences, calculated level positions are given because they are considered more accurate than the measurements presently available. Ionization energies for each ion are derived either from Rydberg series, extrapolation, or calculation. Complete references are given for the compiled data.

Reprint Packages

Package	No.	Title and Contents of Package
C1	5	Molecular Vibrational Frequencies Reprint Nos. 103, 129, 170, 257 and NSRDS 39
C2	22	Atomic Energy Levels Reprint Nos. 26, 54, 64, 68, 94, 100, 109, 125, 126, 131, 132, 149, 150, 154, 156, 160, 179, 180, 192, 200, 222, 278
C3	6	Atomic Spectra Reprint Nos. 33, 56, 77, 78, 110 and 132
C4	5	Atomic Transition Probabilities Reprint Nos. 20, 63, 82, 118 and 182
C5	7	Molecular Spectra Reprint Nos. 4, 8, 53, 79, 93, 130 and 146
C6	9	Thermodynamic Properties of Electrolyte Solutions Reprint Nos. 15, 95, 111, 151, 152, 174, 184, 185 and 186
C7	12	Ideal Gas Thermodynamic Properties Reprint Nos. 30, 42, 43, 62, 65, 66, 70, 80, 83, 113, 115 and 141
C8	7	Resistivity Reprint Nos. 138, 139, 155, 221, 258, 259 and 260
C9	7	Molten Salts Reprint Nos. 10, 41, 71, 96, 135, 167, 168
C10	4	Refractive Index Reprint Nos. 81, 158, 162 and 240

NBS Standard Reference Database 1

NBS/NIH/EPA/MSDC Mass Spectral Database, NBS Standard Reference Database 1, Washington, DC; NBS Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

This database contains electron ionization mass spectra of more than 42,000 different compounds. The spectra were formed by the merger of MSDC and NIH/EPA collections and subsequent removal of all duplicate spectra. Every spectrum has a "Quality Index" associated with it; and for every compound the Chemical Abstracts Service (CAS) name, the molecular weight and formula and the CAS Registry Number is supplied.

NBS Standard Reference Database 2

NBS Chemical Thermodynamics Database, NBS Standard Reference Database 2, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

This database contains recommended values for selected thermodynamic properties for more than 15,000 inorganic substances. These properties include enthalpy of formation from the elements in their standard states, Gibbs energy of formation from the elements in their standard states, entropy, enthalpy content and heat capacity at constant pressure at 298.15 K and 1 atm or 1 bar. Also enthalpy of formation at 0 K is included.

NBS Standard Reference Database 3

NBS Crystal Data Identification File, NBS Standard Reference Database 3, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Lease agreements obtained from JCPDS 1601 Park Lane, Swarthmore, PA (215) 328–9400.

This file contains crystallographic information useful to characterize more than 60,000 different crystalline materials. The data include the reduced cell parameters, reduced cell volume, space group number and symbol, the calculated density, classification by chemical type, chemical formula, and chemical name. Each entry has an associated literature reference.

NBS Standard Reference Database 4

Thermophysical Properties of Hydrocarbon Mixtures (TRAPP), NBS Standard Reference Database 4, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

This database consists of computer software which will predict certain thermophysical properties, namely, density, viscosity, and thermal conductivity for hydrocarbon mixtures. The model used is valid over the entire range of pressure and temperature conditions and covers molecular weight ranges up to C_{20}. The method of calculating is applicable to a wide variety of chemical types, to thermodynamic states ranging from the dilute gas to compressed liquid, and to multicomponent systems.

NBS Standard Reference Database 7

Electron and Positron Stopping Powers of Materials, NBS Standard Reference Database 7, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

This database, also known as EPSTAR, contains data related to the electron and positron stopping powers of various materials. Included in EPSTAR are collision, radiative, and total stopping powers; ranges; radiation yields; and auxiliary information Data are included for electrons in 285 materials, and for positrons in 29 materials, at energies from 10 keV to 10 GeV.

NBS Standard Reference Database 8

X-Ray and Gamma-Ray Attenuation Coefficients and Cross Sections, NBS Standard Reference Database 8, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

This database, also called XGAM, provides photon cross sections (interaction coefficients) and attenuation coefficients for any substance. Interactive software is provided which enables the user to obtain data by entering chemical formulas for a mixture of component materials. The user may also select the energy range over which data are desired. The system operates from a database of cross sections for coherent and incoherent scattering, photoionization and pair production for the elements $Z = 1$ to 100 at energies from 1 keV to 100 GeV.

NBS Standard Reference Database 9

Activity and Osmotic Coefficients of Aqueous Electrolyte Solutions, NBS Standard Reference Database 9, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

This database, called GAMPHI, can be used to calculate values of the mean ionic activity coefficients ($Y_{\pm}$) and the osmotic coefficient of 350 aqueous binary electrolyte solutions at 298.15 K.

NBS Standard Reference Database 10

Thermophysical Properties of Water, NBS Standard Reference Database 10, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

This database calculates the thermodynamic and transport properties of fluid H_2O (liquid and vapor) using the formulation as approved by the International Association for the Properties of Steam (IAPS) at its Tenth International Conference in 1984. The range approved by IAPS for this formulation includes temperatures from 0 to 1000 °C and pressures up to 1500 MPa.

NBS Standard Reference Database 11

DIPPR Data Compilation of Pure Compound Properties, NBS Standard Reference Database 11, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

The DIPPR database contains data on 39 properties for 346 chemical compounds. These data were released for public distribution by the Design Institute for Physical Property Data (DIPPR). For each chemical compound included, values are given for 26 single-valued property constants and for 13 properties as functions of temperature, calculated from correlation coefficients. The database also includes estimates of the accuracy of each property value and references to the sources of measured or predicted data which were used in selecting the recommended values.

NBS Standard Reference Database 12

Interactive FORTRAN Program to Calculate Thermophysical Properties of Fluids MIPROPS, 1986, NBS Standard Reference Database 12, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

This program computes thermophysical properties of twelve fluids: helium, argon, parahydrogen, oxygen, nitrogen, nitrogen trifluoride, ethylene, methane, ethane, propane, isobutane and normal butane. Properties are computed for the single phase region from input of two of the following variables: temperature, pressure, and density. Values on the liquid-vapor boundary are computed for either a given temperature and pressure.

NBS Standard Reference Database 13

JANAF Thermochemical Tables, NBS Standard Reference Database 13, Washington, DC; NBS, Office of Standard Reference Data, (updated periodically). Call (301) 975–2208 for specific instructions.

The JANAF Thermochemical Tables provide a compilation of critically evaluated thermodynamic properties of approximately 1,800 substances over a wide range of temperature. Recommended temperature-dependent values are provided for chemical thermodynamic properties of inorganic substances and for organic substances containing only one or two carbon atoms. These tables cover thermodynamic properties over a wide temperature range with single-phase and multiphase tables for crystal, liquid, and ideal gas state.

NSRDS-NBS Series

3 Sec. 11

Selected Tables of Atomic Spectra: A. Atomic Energy Levels - Second Edition; B. Multiplet Tables; O III—Charlotte E. Moore. NSRDS-NBS 3, 33 p. (1985).

This publication is the eleventh section of a series being prepared in response to the need for a current revision of two sets of the author's tables containing data on atomic spectra as derived from analyses of optical spectra.

NBS Technical Notes

1097

Interactive FORTRAN Program for Micro Computers to Calculate the Thermophysical Properties of Twelve Fluids (MIPROPS) — Robert D. McCarty. NBS Tech. Note **1097**, 84 p. (1986).

The thermophysical and transport properties of selected fluids have been programmed in FORTRAN 77 which is available for micro computers. The input variables are any two (pressure, density, and temperature) in the single phase region and either pressure or temperature for the saturated liquid or vapor states. The output is pressure, density, temperature, internal energy, enthalpy, entropy, specific heat capacities, speed of sound, and, in most cases, viscosity, thermal conductivity and dielectric constant. The fluids included are: helium, hydrogen, nitrogen, oxygen, argon, nitrogen trifluoride, methane, ethylene, ethane, propane, iso- and normal butane.

1206

GAMPHI-A Database of Activity and Osmotic Coefficients for Aqueous Electrolyte Solutions—R. N. Goldberg, J. L. Manley, R. L. Nuttall. NBS Tech. Note **1206**, 23 p. (1985).

This publication concerns a database of activity and osmotic coefficients for 350 binary aqueous electrolyte solutions at 298.15 K together with a collection of subroutines for utilizing the database. The codes, which are written in FORTRAN 77, can be used either interactively or individual subroutines can be referenced via FORTRAN CALL statements from user-written programs.

1208

PIPE/1000: An Implementation of Piping on an HP-1000 Minicomputer— N. L. Seidenman. NBS Tech. Note **1208**, 23 p. (1985).

This paper describes an implementation of piping in on an HP-1000 minicomputer. Piping is a system by which programs can communicate so as to coordinate their respective functions in a synchronized effort aimed at the completion of a given task.

NBS Special Publications

689

Computerizing Materials Data-A Workshop for the Nuclear Power Industry — John Rumble, Jr. and Jack H. Westbrook. NBS Spec. Publ. **689**, 37 p. (1985).

This publication details the conclusions and recommendations of a workshop attended by scientists and engineers responsible for the use of materials property data in various sectors of the nuclear power industry. At this workshop, all facets of the use of computers in accessing these data were addressed. The discussions concerned the content of a proposed computerized materials data system, its size and data sources, and the user interfaces and system capabilities.

702

Standards and Metadata Requirements for Computerization of Selected Mechanical Properties of Metallic Materials— Jack H. Westbrook. NBS Spec. Publ. **702**, 39 p. (1985).

This publication concerns a computerized information system on the engineering properties of materials, the standards and metadata requirements for a representative group of mechanical property categories. These categories include: tensile behavior, hardness numbers, notch-bar impact test parameters and fatigue properties. For each property group, definition of terms, synonyms (and non-synonyms), standard test methods, standards for reporting data, precision and accuracy, and correlations of properties are addressed.

708

Standard Reference Data Publications 1964–1984, — Joan C. Sauerwein and Geraldine R. Dalton. NBS Spec. Publ. **708**, 138 p. (1985).

This document provides a comprehensive list of the products available from the National Standard Reference Data System (NSRDS) for the the years 1964–1984, including indexes qualified by author, material, and property terms.

726

Materials Information for Science and Technology (MIST): Project Overview Phase I and II and General Considerations—Walter Grattidge, Jack Westbrook, John McCarthy, Clyde Northrup, Jr., John Rumble, Jr. NBS Spec. Publ. **726**, 118 p. (1986).

The National Bureau of Standards and the Department of Energy have embarked on a program to build a demonstration computerized materials data system called Materials Information for Science & Technology (MIST). This report documents the first two phases of the project as well as setting forth many general considerations that will shape later phases.

NBS Interim Reports

85-3205

Chemical Thermodynamics in Steam Power Cycles Data Requirements — Otaker Jonas and Howard J. White, Jr. NBSIR **85-3205**, 282 p. (1985).

A workshop on the needs for chemical thermodynamic data in steam power cycles was held at the National Bureau of Standards in Gaithersburg, Maryland, February 8–9, 1983. In these proceedings, the purpose of the workshop is presented and the principal conclusions and recommendations are stated. The texts or principal conclusions and recommendations are also given.

NSRDS Data Publications from Other Publishers

Binary Alloy Phase Diagrams — Thaddeus B. Massalski (editor). American Society for Metals, Metals Park, OH, 2224 p. (1986).

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Bulletin of Alloy Phase Diagrams — Joanne L. Murray (editor). Bull. Alloy Phase Diag. **6**, Metals Park, OH: American Society for Metals, (1985).

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Mossbauer Effect Reference and Data Journal—J. G. Stevens, V. E. Stevens, R. M. White, J. L. Gibson, (editors). Moss. Eff. Ref. Data J. 8, Asheville, NC: Mossbauer Effect Data Center, U. of NC, (1985).

Mossbauer Effect Reference and Data Journal—John G. Stevens, Virginia E. Stevens, Mary Alice Goforth, Janet L. Gibson, Pamela C. Newman, (editors). Moss. Eff. Ref. Data J. 9, Ashville, NC: Mossbauer Effect Data Center, U. of NC, (1986).

Biweekly List of Papers on Radiation Chemistry and Photochemistry Vol. 18. 1985—Rad. Chem. 18, Notre Dame, IN: Radiation Chem. Data Center, U. of Notre Dame, 35 p. (1985). $30.00; the Biweekly List, Vol. 17 (1984) plus the Annual Cumulation, $45.00, foreign and airmail postage rates available upon request.

Biweekly List of Papers on Radiation Chemistry and Photochemistry, Annual Cumulation with Keyword and Author Indexes, Vol. 18. 1985—Rad. Chem. 18, Notre Dame, IN: U. of Notre Dame, 490 p. (1985). $30.00; the Biweekly List, Vol. 18 (1985) plus the Annual Cumulation, $45.00, foreign and airmail postage rates available upon request.

Biweekly List of Papers on Radiation Chemistry and Photochemistry Vol 19, 1986—Rad. Chem. 19, Notre Dame, IN: Radiation Chem. Data Center, U. of Notre Dame, 35 p. (1986). $30.00; the Biweekly List, Vol. 18 (1985) plus the Annual Cumulation, $45.00, foreign and airmail postage rates available upon request.

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Energy, dissociation

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Mobility of electrons and holes
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