

National Bureau of Standards

*Compiled Thermodynamic Data  
Sources for Aqueous and  
Biochemical Systems:  
An Annotated Bibliography (1930-1983)*

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The National Bureau of Standards<sup>1</sup> 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 and provides: (1) a basis for the nation's physical measurement system, (2) scientific and technological services for industry and government, (3) a technical basis for equity in trade, and (4) technical services to promote public safety. 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 Center for Materials Science.

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- Chemical Physics
- Analytical Chemistry

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Provides technology and technical services to the public and private sectors to address national needs and to solve national problems; conducts research in engineering and applied science in support of these efforts; builds and maintains competence in the necessary disciplines required to carry out this research and technical service; develops engineering data and measurement capabilities; provides engineering measurement traceability services; develops test methods and proposes engineering standards and code changes; develops and proposes new engineering practices; and develops and improves mechanisms to transfer results of its research to the ultimate user. The Laboratory consists of the following centers:

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- Manufacturing Engineering
- Building Technology
- Fire Research
- Chemical Engineering<sup>2</sup>

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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-country 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 Center consists of the following Divisions:

- Inorganic Materials
- Fracture and Deformation<sup>3</sup>
- Polymers
- Metallurgy
- Reactor Radiation

<sup>1</sup>Headquarters and Laboratories at Gaithersburg, MD, unless otherwise noted; mailing address Gaithersburg, MD 20899.

<sup>2</sup>Some divisions within the center are located at Boulder, CO 80303.

<sup>3</sup>Located at Boulder, CO, with some elements at Gaithersburg, MD.

*NBS Special Publication 685*

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### ABSTRACT

This is a selected and annotated bibliography of sources of compiled and evaluated chemical thermodynamic data relevant to biochemical and aqueous systems. The principal thermodynamic properties considered herein are Gibbs energy and equilibrium data, enthalpies of formation and reaction, heat capacities and entropies, and the corresponding partial molar and excess properties. Derived quantities used in calculating the above are also included. Transport and mechanical data have also been identified to a lesser degree. Included in the annotations to the data sources are brief descriptions of the types of properties tabulated, the classes of materials dealt with, and the degree of completeness of the compilations.

Keywords: Aqueous systems; bibliography; biochemical systems; enthalpy data; entropy data; equilibrium data; excess properties; Gibbs energy data; heat capacity data; partial molar properties; review articles; thermochemistry; thermodynamics.

## INTRODUCTION

"There is a growing need for reliable thermodynamic data for both scientific and practical purposes. However, the existence of a desired piece of data in the primary literature does not guarantee its recovery by an interested user. Indeed the recovery process may be a decidedly non-trivial as well as a time consuming matter. At one time this problem was, in large part, managed by periodic review articles, monographs, and the International Critical Tables. The National Standard Reference Data System, CODATA, and other coordinating organizations are helping to provide current compilations. However, the preparation of new reviews is sufficiently complex that there are at any give time many subject areas that do not have current compilations available. In this circumstance earlier reviews are an important resource for the technologist or scientist. Unfortunately, the proliferation of such works and the enormity of the available literature have made even the recovery of review and compilation articles a matter of some difficulty. It is to help solve this problem for one small part of our science that we have prepared this annotated bibliography of thermodynamic data sources relevant to biochemical and aqueous systems. These two areas are mutually complementary. In environmental problems such as water quality control, and in the utilization of aqueous systems with respect to energy resources and the processing of material resources, the aqueous systems of interest very often include the same substances and require the same information as in the study of biochemical systems. In addition to information on the aqueous solutions, the properties of the pure substances are often required in order to establish reference points for interrelating various systems. Thus, this bibliography is a selective listing of sources of thermodynamic information for pure substances and aqueous solutions, selected for their particular relevance to these kinds of problems."

The above quotation is from NBS Special Publication 454 and it contains the principle upon which both that publication and this one, the successor to it, are based. The identification and collection of sources of compiled thermodynamic data was begun by the late George Armstrong at the National Bureau of Standards at least ten years ago. The author joined him in this task several years ago and with him co-authored NBS Special Publication 454 on this subject in 1976. Many of the descriptions of older works in this Bibliography are taken directly from Special Publication 454. The intervening years have seen a remarkable growth in the subject matter of this Bibliography and a revision of it was suggested by the Design Institute for Physical Property Data of the American Institute of Chemical Engineers which also helped in providing the necessary funding for the project. A "review of reviews" which the reader might also wish to consult is the chapter by E. F. G. Herrington in "Chemical Thermodynamics: Volume I" (see item [90]).

The scope of the present work remains essentially that of Special Publication 454. The general aim is to assist the reader in locating those publications which contain thermochemical data which can best serve his needs. Equilibrium data is taken in its most general sense and includes equilibrium constants, enthalpies, entropies, heat capacities, volumes, and partial molar and excess property data. To a much lesser extent, transport and other properties have been included. Unfortunately, much of the data on biochemical systems is scattered throughout much of the literature and there is a need for

definitive reviews and compilations in several areas such as enzyme-catalyzed reactions and on the denaturation of enzymes and nucleic acids. This need is all the more pressing due to the growing importance of bio-engineering and its industrial importance. Because of this, various chapters and short reviews in books on biochemistry have been included in this bibliography.

The entries are listed in alphabetical order by first author or by the editor. There are a few cases in which the work of a research group, or the volumes of a multi-volume work are kept together and entered under the name of the principal researcher, the editor, or the institution. All authors have been cited in the author index and it should be consulted if an article is not found where expected.

Each annotation contains a brief summary of the contents of the book or article cited. Specifically, the nature and state of the substances dealt with, the extent of coverage, and whether the given property values have been compiled, selected, or critically evaluated is stated. Also, whenever a meaningful statement on temperature range can be made, it has been included. For some large compilations the ranges are too different for individual systems to make any statement practical, and for them, the authors have usually attempted to cover the full range of the data. It is hoped that the contents of the annotation is sufficient to permit the reader to select those references which most directly apply to his own needs.

The present bibliography identifies 162 different sources for the reader to consult. Unfortunately, many of the books cited are out-of-print, not in English, or in report form (many of the U.S. government sponsored reports are available from the National Technical Information Service, Springfield, Virginia 22161). The reader is urged to exercise care and judgment when combining formation properties from different sources when calculating equilibrium constants and enthalpies of reaction. There are several reasons for this precaution: (1) different reference states may be used for the elements, (2) there are different conventions regarding standard states, (3) equilibrium "constants" may be concentration dependent, and (4) different thermodynamic pathways may have been used to calculate tabulated formation properties. The safest approach here is to calculate equilibrium constants (or enthalpy and entropy changes) from the formation properties given in one reference and then to combine them with similar data calculated or found in other references.

The alphabetical subject index that follows the main section of this bibliography gives an indication of thermodynamic properties, physical or chemical processes, classes of substances, and, in a few cases, individual substances for which information is to be found herein. It is not practical to give an exhaustive index to the contents of the individual references. Hence the absence of a piece of information in the index does not necessarily mean its absence in the references. This is particularly true with respect to particular substances, which the reader should assume are not listed except by chance of title or abstract.

It is not possible to claim completeness for this bibliography and somewhat arbitrary decisions have been made as to whether or not to include a specific item. The author would appreciate comments from interested readers concerning data sources omitted from this bibliography.

The author thanks Drs. William Evans, David Garvin, and Vivian Parker for their comments on this bibliography and Beverly S. Geisbert for her excellent clerical work on the manuscript.



BIBLIOGRAPHY

- [1] Alberty, R. A.  
Standard Gibbs Free Energy, Enthalpy, and Entropy Changes as a Function of pH, and pMg for Several Reactions Involving Adenosine Phosphates  
Journal of Biological Chemistry 244, 3290 (1969).

The standard Gibbs energy, enthalpy, and entropy changes for the hydrolysis of adenosine-5'-triphosphate to adenosine-5'-diphosphate are computed as a function of pH and magnesium ion concentration at 25 °C. A critical evaluation of the relevant literature data is included. Also see item [120]

\* \* \* \* \*

- [2] Armstrong, G. T., Domalski, E. S., Furukawa, G. T., Reilly, M. L., Wilhoit, R. C. and others  
A Survey of Thermodynamic Properties of the Compounds of the Elements CHNOPS - A Series of Eighteen Reports  
(National Bureau of Standards Reports No. 8521, 8595, 8641, 8906, 8992, 9043, 9089, 9374, 9449, 9501, 9553, 9607, 9883, 9968, 10070, and 10291, published during the years 1964 to 1970, U. S. Department of Commerce, Washington, D.C.)

This series of reports is a survey of the thermodynamic properties of selected compounds of biological importance containing the elements carbon, hydrogen, nitrogen, oxygen, phosphorus, and sulfur. Included in these reports are heat capacity data; heats and Gibbs energies of formation; vapor pressure data; tables of thermodynamic functions; Gibbs energies, entropies and enthalpies of solution and dilution; and thermodynamic properties of mixed solvent systems. Except for the tables of thermal functions, the data refer to 25 °C or nearby temperatures. References to sources of data in the literature are included.

Some of the data contained in these reports formed the basis of Domalski's enthalpy of combustion tables (see item [29]) and of Wilhoit's tables (see item [15]). The remainder of the material in these reports has not appeared in press elsewhere. The NBS Chemical Thermodynamics Data Center has a complete set of these reports available for examination.

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- [3] Ashcroft, S. J. and Mortimer, C. T.  
Thermochemistry of Transition Metal Complexes  
(Academic Press, London and New York, 1970).

This book surveys the literature to 1968 on energy changes for processes involving transition metal complexes including both organic and inorganic ligands. A critical review of the thermochemical data for over 1500 systems of complexes is given. Comparable data from various sources are shown in juxtaposition. Values of  $\Delta H$ ,  $\Delta G$ , and  $\Delta S$  for various stages of complex formation are usually listed for processes in aqueous solution at or near 25 °C.  $\Delta_f H^\circ$ ,  $\Delta_f G^\circ$ ,  $\Delta_f S^\circ$  for crystalline complex substances are given where available. In many instances correlations of the data for various metals with a single ligand, and for various related complexes of a given metal, are given graphically or by means of bond-energy estimates based on the data.

\* \* \* \* \*

- [4] Baes, C. F., Jr. and Mesmer, R. E.  
The Hydrolysis of Cations  
(John Wiley and Sons, New York, 1976)

This book on the chemistry of hydrolysis of inorganic cations contains a substantial amount of equilibrium data pertinent to hydrolysis reactions. For each of the elements which produces a cation or cations in aqueous solution, the available equilibrium data for the hydrolysis reaction(s) at or about 298 K has been critically assessed in order to obtain "best" values for equilibrium constants and quotients applicable to a given medium. When available,  $\Delta H$  and  $\Delta S$  data for the hydrolysis reactions are also presented. The data, with references and comments, is arranged under the element of interest.

\* \* \* \* \*

- [5] Barner, H. E. and Scheurman, R. V.  
Handbook of Thermochemical Data for Compounds and Aqueous Species  
(John Wiley and Sons, New York, 1978)

This book presents thermodynamic properties for a wide variety of ions and complexes in aqueous solution over a range of temperature (typically 25 to 300 °C). Most of the properties were calculated from data at 25 °C, much of which was taken from the National Bureau of Standards Technical Note 270 (see item [149]). Phase transition data were taken from the book by I. Barin and O. Knacke, "Thermochemical Properties of Inorganic Substances" (Springer-Verlag, Berlin, 1973). The extension of the 25 °C data to higher temperatures was done using estimation schemes such as those developed by C. M. Criss and J. W. Cobble (J. Am. Chem. Soc. 86, 5390 (1964)) and H. C. Helgeson (J. Phys. Chem. 71, 3121 (1967)).

\* \* \* \* \*

- [6] Bates, R. G.  
Determination of pH, Theory and Practice (Second Edition)  
(John Wiley and Sons, New York, 1973)

This book, the primary topic of which is the establishment of an operational pH scale, contains several tables of interest. Tabulated are the ion product of water from 0 to 60 °C, the vapor pressure, density, and dielectric constant of water from 0 to 100 °C, dielectric constants of pure liquids, and pH values of several aqueous buffer systems.

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- [7] Battino, R.  
Volume Changes on Mixing for Binary Mixtures of Liquids  
Chemical Reviews 71, 5 (1971).

This critical and extensive review deals with both the volume changes associated with the mixing of binary mixtures of liquids and partial molar volumes at infinite dilution of various solvent systems, aqueous and non-aqueous. The temperature range cited is that at which the experimental measurements have been performed. Included is a detailed discussion of the experimental methods used for measurements and associated theoretical developments. The coverage

of the available literature appears to be very thorough. There are 427 references to the primary literature.

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- [8] Battino, R., and Clever, H. L.  
The Solubility of Gases in Liquids  
Chemical Reviews 66, 395 (1966)

This thorough and detailed review contains a discussion of experimental methods for the measurement of gas solubilities in all types of liquids, including water. Tabulated are the solubilities of oxygen, nitrogen, and argon in water at one atmosphere pressure and from 0 to 50 °C. Also to be found herein is an extensive table listing sources of gas solubility data in the primary literature. Although the tables do not give selected values, the authors have given their assessment of the reliability of the data to be found in the listed sources by means of a coding scheme. There are 686 references to the primary literature. Also see item [154].

\* \* \* \* \*

- [9] Beezer, A. E. (editor)  
Biological Microcalorimetry  
(Academic Press, London and New York, 1980)

This book contains fourteen chapters on various topics related to calorimetry as applied to biochemical and biological systems. The coverage of topics is very broad and includes bacteria, cells, microorganisms, drugs, membranes, and enzymes. While there are few tables of thermodynamic data in this book, many of the chapters contain useful collections of references to the literature pertinent to the topic of the individual chapter.

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- [10] Benson, S. W.  
Thermochemical Kinetics:  
Methods for the Estimation of Thermochemical Data and Rate Parameters  
(Second Edition)  
(John Wiley and Sons, New York and London 1976)

This monograph gives tables of necessary data and descriptions of methods of their use for calculating  $\Delta H_f^\circ$ ,  $C_p$ , and  $S$  at 25 °C for gas phase molecules and radicals and for extrapolating them to higher temperatures. The procedures can be applied to hydrocarbons, oxygen-containing compounds, nitrogen-containing compounds, polycyclic structures, haloalkanes, organo-sulfur compounds, organo-metallic compounds, polycyclic substances, and deal principally with organic compounds.

\* \* \* \* \*

- [11] Benson, S. W., Cruickshank, F. R., Golden, D. M., Haugen, G. R.,  
O'Neal, H. E., Rogers, A. S., Shaw, R. and Walsh, R.  
Additivity Rules for the Estimation of Thermochemical Properties  
Chemical Reviews 69, 279 (1969)



This lengthy technical article gives procedures for calculating the properties  $\Delta_f G^\circ$ ,  $S^\circ$ ,  $C_p^\circ$ , for organic compounds in the gas phase. Parameters for calculating  $C_p^\circ$  are given for the temperature range from 300 to 1500 K. The availability of  $C_p^\circ$  as a function of temperature allows calculation of  $\Delta_f G^\circ$  and  $S^\circ$  at the same temperatures. The necessary constants for making the calculations are given for individual chemical groupings in some 38 tables. Many classes of functional groups and molecular conformations are included. Examples are given comparing calculated and observed values. Agreements of 1 kcal·mol<sup>-1</sup> (4.184 kJ·mol<sup>-1</sup>) or better in  $\Delta_f G^\circ$  and 1 cal·mol<sup>-1</sup>·K<sup>-1</sup> or better in  $C_p^\circ$  and  $S^\circ$  are generally found. Also see item [10] which supersedes this article.

\* \* \* \* \*

- [12] Bichowsky, F. R. and Rossini, F. D.  
The Thermochemistry of the Chemical Substances  
(Reinhold Publishing Corporation, New York, 1936)

Although outdated, this book still provides useful references to the older thermochemical literature. Tabulated are  $\Delta_f H^\circ$  and enthalpy of transition values for the elements and their compounds, with the data for carbon-containing compounds being terminated at two carbon atoms. It should be noted that the data pertain to a temperature of 18 °C and to diamond, rather than graphite, as the standard state for carbon; the yellow form is the reference state for phosphorus. The yellow form is thermochemically identical to the white form which is the reference state used in the NBS Thermochemical Tables [149]. The data upon which this book was based were used in preparing NBS Circular 500, see item [131].

\* \* \* \* \*

- [13] Bondi, A.  
Physical Properties of Molecular Crystals, Liquids, and Glasses  
(John Wiley and Sons, New York and London, 1968)

This monograph is designed for use by chemical engineers in estimating physical properties needed in design calculations, as well as by physical chemists and synthetic chemists who need to understand the relationship between structure and physical properties. Correlations of several kinds are described in the text. These are then restated as methods for estimation of the properties.

Substances considered include non-polar and polar gases, non-polar and polar liquids, associated liquids, crystalline solids, glasses, polymers, and polymer melts, as well as others. Procedures given include many variants, depending upon the properties given as initial information. Among the properties for which procedures are given are: density, heat capacity, enthalpy, entropy, enthalpy and entropy of fusion, enthalpy of vaporization, vapor pressure, cubical thermal expansion coefficient, bulk modulus, Young's modulus compressibility, thermal conductivity, rotational diffusion constant, relaxation times, mass diffusion, viscosity, and others.

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- [14] Boublik, T., Fried, V. and Hala, E.  
The Vapour Pressures of Pure Substances  
(Elsevier, New York, 1973)

Data are presented in the form of constants for the Antoine equation for the temperature dependence of the vapor pressures of 806 substances in the normal and low pressure region. Almost all of the substances contain carbon. Experimental data from selected original sources are given, together with smoothed values obtained from the Antoine equations at the same temperature, and the absolute and percentage deviations. Standard deviations are calculated. A standard boiling point is calculated for each substance.

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- [15] Brown, H. D. (editor)  
Biochemical Microcalorimetry  
(Academic Press, New York and London, 1969)

This book contains seventeen chapters on subjects concerning heat measurements and their relationship to biology and biochemistry. Also see the 1980 volume of this same series, item [63]. Several of the articles contain tabulations of data:

Author(s)

Title of Chapter

R. C. Wilhoit

Thermodynamic Properties of Biochemical  
Substances

This chapter (no. II) includes several tables: (1) Selected values of thermodynamic properties ( $\Delta_f G^\circ$ ,  $\Delta_f H^\circ$ ,  $S^\circ$ , and  $C_p^\circ$ ) for about 120 important biochemical species or compounds; (2) Enthalpies and Gibbs energies of formation of adenosine phosphoric acid species relative to  $H_2ADP^{1-}$  at 25 °C; (3)  $\Delta H^\circ$  and  $\Delta G^\circ$  for six important biochemical processes; and (4) Partial molar properties ( $L_2$ ,  $L_1$ ,  $C_1$ ) of aqueous glucose, glycerol, glycine, and urea at 25 °C.

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S. Ono and K. Takahashi

Chemical Structure and Reactions of Carbohydrates

This chapter (no. IV) has a table of enthalpies of isomerization of eleven carbohydrates and a table given enthalpies of hydrolysis of aqueous  $\alpha$ -1,4 and  $\alpha$ -1,6 glucosidic linkages in several glucosides at 25 °C.

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T. Ackermann

Physical States of Biomolecules: Calorimetric  
Study of Helix-Random Coil Transitions in Solution

This chapter (no. VI) contains a tabulation of calorimetrically determined enthalpy values accompanying conformational changes of macromolecules in solution (26 references) and their transition temperatures.

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This chapter (no. VII) contains a summary of calorimetric enthalpy values for enzyme catalyzed systems (21 references) at or near 25 °C.

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- [16] Chapman, T. W. and Newman, J.  
A Compilation of Selected Thermodynamic and Transport Properties of  
Binary Electrolytes in Aqueous Solution  
(U. S. Atomic Energy Commission Report UCRL-17767 (1968))

Data from the literature on the properties of sixty-one common binary inorganic electrolytes at various temperatures are tabulated with appropriate references. The properties include the density, viscosity, transference number, diffusion coefficient, and the activity coefficient.

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- [17] Charlot, G.  
Selected Constants - Oxidation-Reduction Potentials of Inorganic Substances  
in Aqueous Solution  
(Butterworths, London, 1971)

This reference work, prepared under the auspices of the IUPAC, contains selected values of electrochemical potentials relative to the assigned zero value of the standard hydrogen electrode at or near 25 °C. Entries are given for about 350 inorganic systems. The literature coverage is through 1967.

\* \* \* \* \*

- [18] Christensen, J. J., Eatough, D. J. and Izatt, R. M.  
Handbook of Metal Ligand Heats and Related Thermodynamic Quantities  
(Second edition)  
(Marcel Dekker, New York, 1975)

This handbook gives tabulated values of thermodynamic functions in aqueous solution. Enthalpies are given for equilibria involving metal ions and ligands, together with the related thermodynamic quantities  $\log K$ ,  $\Delta S$ , and  $\Delta C_p$ , where available. The body of the book consists of a table (414 pp.) in which are summarized the published literature values up to 1974, classified according to ligand. In addition, the appropriate reaction, the method, and conditions of measurement of  $\Delta H$  are given. The temperatures are also specified and are in the vicinity of 25 °C. Both inorganic and organic ligands, and complexes of about seventy metallic elements are given. A seven page guide to the use of the table and indexes is given. The table is indexed by author, by ligand formula, and by metal. An index of synonyms and a chronological list of references are also given.

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- [19] Christensen, J. J., Eatough, D. J. and Izatt, R. M.  
The Synthesis and Ion Binding of Synthetic Multidentate Macrocyclic  
Compounds  
Chemical Reviews 74, 351 (1974)

This review article contains, in addition to a discussion on the synthesis, kinetic, and structural parameters, a referenced compilation of  $\log K$ ,  $\Delta H$ ,  $\Delta S$ , and  $\Delta C_p$  data at or near 25 °C for the interaction of inorganic cations with synthetic multidentate macrocyclic compounds. Each entry in the table of thermodynamic data includes the ionic strength, solvent system, and method of measurement used in obtaining the data.

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- [20] Christensen, J. J., Hansen, L. D. and Izatt, R. M.  
Handbook of Proton Ionization Heats and Related Thermodynamic Quantities  
(John Wiley and Sons, New York, 1976)

This book is a compilation of enthalpies, entropies, and  $pK$  values for the proton ionization of (mostly) organic compounds in water. For each of the approximately 600 compounds covered in this handbook is given the  $\Delta H$ ,  $\Delta S$ , and  $pK$  for the proton ionization, the method and conditions of measurement, and some brief remarks. The temperatures are also specified and are at or near 25 °C. Literature references are also given for each compound.

\* \* \* \* \*

- [21] Clark, W. M.  
Oxidation-Reduction Potentials of Organic Systems  
(The Williams and Wilkins Company, Baltimore, 1960)

This 584 page monograph contains a comprehensive discussion on the determination of the electrochemical potentials of organic systems with emphasis both on theory and experimental practice. Included are approximately 100 tables of critically evaluated oxidation and reduction potentials for organic and biochemical systems through about 1960. Included are the quinones, phenols, anilines, porphyrins, nicotinamide-adenine dinucleotide, and nicotinamide-adenine dinucleotide phosphate systems, and several others. The author has, in most cases, specified the conditions to which the data refer.

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- [22] Clarke, E. C. W. and Glew, D. N.  
Journal of the Chemical Society Faraday Transactions I 76, 1911 (1980)

Debye-Hückel limiting slopes for the osmotic coefficient in water are presented as a function of temperature (0 to 150 °C). The recommended values were derived from literature measurements of the static dielectric constant and density of water.

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- [23] CODATA Recommended Key Values for Thermodynamics 1977  
(CODATA Bulletin No. 28 (1978) and Tentative Set of Key Values for Thermodynamics: Parts VI, VII, and VIII, CODATA Special Reports: No. 4 (March 1977), No. 7 (April 1978), and No. 8 (April 1980))  
(CODATA Secretariat, Paris)

These are reports by the CODATA (Committee on Data for Science and Technology of the International Council of Scientific Unions) Task Group on Key Values for Thermodynamics in which are presented recommended values for the quantities  $\Delta_f G^\circ$  (298.15 K),  $S^\circ$  (298.15 K),  $\Delta_f H^\circ$  (298.15 K), and  $H^\circ$  (298.15 K) -  $H^\circ$  (0 K) for  $\approx 180$  of the thermochemically more important elements and compounds, including some aqueous species, mostly electrolytes. These bulletins supersede earlier CODATA reports of this group. The recommended values are based on a completely new evaluation of all pertinent data available at the time of publication. Consequently, they should not be used indiscriminately with data from earlier self-consistent tables, such as Wagman et al. or Medvedev et al., items [93] and [149]. The earlier publications in this series include CODATA Bulletins 5, 10, 17, and 22 published, respectively, in 1971, 1973, 1976, and 1977. They are useful for the references which they contain to the source literature from which the recommended key values were obtained.

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- [24] Coetzee, J. F. and Ritchie, C. D. (editors) (in two volumes)  
Solute-Solvent Interactions  
(Marcel-Dekker, New York and London, 1969 and 1976).

Relevant chapters are:

<u>Author(s)</u>	<u>Title of Chapter</u>
J. W. Larson and L. G. Hepler	Heats and Entropies of Ionization (Vol 1, Chapter 1)

This is a detailed review and evaluation of the enthalpies, Gibbs energies, entropies, and heat capacity changes accompanying ionization of organic acids. Included are eleven tables of data on various types of acids, including the carboxylic acids, phenols, anilinium ions, ammonium ions, the amino acids, barbituric acids, and several inorganic acids. The authors also discuss the interpretation of the data in terms of molecular considerations. The tabulated data refer to 25 °C and standard state conditions. There are 224 references.

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E. M. Arnett and D. R. McKelvey	Solvent Isotope Effect on Thermodynamics of Non-reacting Solutes (Vol. 1, Chapter 6)
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This is a general and extensive review dealing with differences in thermodynamic properties between light and heavy water systems. The properties dealt with include Gibbs energies and enthalpies of transfer and solubilities; systems for which data are tabulated include the more common inorganic electrolytes and ions, alcohols, amides, amino acids, and several non-electrolytes.

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P. M. Laughton and R. E. Robertson	Solvent Isotope Effects for Equilibria and Reactions (Vol. 1, Chapter 7)
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Included in this review are tabulated values giving differences in pK values for weak acids in light and heavy water.

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C. V. Krishnan and H. L. Friedman    Enthalpies of Transfer for Solutes  
in Polar Solvents (Vol. 2, Chapter 3)

The chapter reviews the existing experimental data for standard enthalpies and entropies of solution of pure substances in various solvents and gives derived entropies of transfer of molecules, ions, and groups from one solvent to another and from the gas phase to water. The data are summarized in 22 tables and cover both inorganic and organic substances, electrolytes and non-electrolytes. There are 146 references to the literature.

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- [25] Cohn, E. J. and Edsall, J. T. (including chapters by J. G. Kirkwood, H. Mueller, J. L. Oncley, and G. Scatchard)  
Proteins, Amino Acids, and Peptides: As Ions and Dipolar Ions  
(Hafner Publishing Co., New York and London, 1965)

This book contains a general discussion of the physical chemistry of proteins, amino acids, and peptides. Most of the chapters contain references to the source literature where one can find specific pieces of thermodynamic data.

Tables in this book of particular interest to this bibliography are:

(1) activity coefficients of amino acids and peptides, (2) solubilities of amino acids in water and other solvents, (3) the influence of  $\text{CH}_2$  groups upon the interactions between dipolar ions, (4) enthalpies of ionization of amino acids and peptides, and (5) thermodynamic functions ( $\Delta G^\circ$ ,  $\Delta H^\circ$ ,  $\Delta S^\circ$ , and  $\Delta C_p^\circ$ ) for the ionization of amino acids. Also see entry [24].

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- [26] Conway, B. E.  
Electrochemical Data  
(Elsevier, New York, 1952)

This monograph is a comprehensive (359 pp.) collection of data on various aspects of pure and applied electrochemistry, relating to organic and inorganic substances, both solid and in solution. Data are presented in tabular form, in ten chapters, introduced with references to data sources and explanations of approach. Physical properties include densities and vapor pressures of various aqueous solutions, dielectric constants, dipole moments, and other properties. Relative partial molar enthalpies and activity and osmotic coefficients, conductance values, ionic mobilities, transference numbers and diffusion coefficients are tabulated. There is a chapter on dissociation constants, solubilities, and buffer solutions. The chapter on properties of electric double layers contains tables of electrokinetic potentials and properties of various interfaces including ones of such biological interest as the mammalian red blood cell. The biologist would also find relevant the section on transport and general properties of colloids and macromolecular electrolytes, including extensive tables of mobilities for such compounds as

hemoglobins, serum albumins, and red blood cells, among others. Electrode chemistry tables include a compilation of data on reversible electrode processes:

liquid junction potentials, half-cell potentials, and electrochemical equivalents for certain elements. A chapter on electrode kinetics gives a critical selection of the available determinations of the parameters of a number of electrode reactions.

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- [27] Covington, A. K.  
Electrolyte Solutions Bulletin  
(University of Newcastle-Upon-Tyne, 1971 to present)

This is a current awareness bulletin that provides titles and references of "recent papers covering all aspects of the physical chemistry and structure of electrolyte solutions, the methods used in these studies including spectroscopy, equilibrium (but not kinetic processes), electrode systems, pH, ion selective and reference electrodes."

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- [28] Cox, J. D. and Pilcher, G.  
Thermochemistry of Organic and Organometallic Compounds  
(Academic Press, London and New York, 1970)

This monograph is a critical compilation of thermochemical data for the title field published since 1930. The enthalpies of formation at 298.15 K of some 3000 substances are listed, with estimates of error. Where enthalpies of vaporization are known or can be reliably estimated these are listed and in these cases the enthalpies of formation of both gaseous and condensed phases are given. Extensive introductory material presents experimental procedures for reduction of experimental data of the type found in the book. Applications of thermochemical data are given, and there is a section on methods of estimating enthalpies of formation of organic compounds. Also see items [29] and [116].

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- [29] Domalski, E. S.  
Selected Values of Heats of Combustion and Heats of Formation of Organic Compounds Containing the Elements C, H, N, O, P, and S  
Journal of Physical and Chemical Reference Data 1, 221 (1972)

Selected values of the enthalpies of combustion and enthalpies of formation of 719 organic compounds at 298.15 K are reported. The selected values are augmented by commentary and original source references. The Wiswesser Line Notation is also given for each compound. The methods used in updating older work are described.

\* \* \* \* \*

- [30] Domalski, E. S., Evans, W. H. and Hearing, E. D.  
Heat Capacity, Entropies, and Some Phase Transition Properties of Organic Compounds in the Liquid and Solid Phases  
Journal of Physical and Chemical Reference Data, Volume 13,  
Supplement No. 1, 1984. (286 pp.)

This extensive review gives heat capacities and entropies for approximately 1400 organic compounds in the liquid and solid phases at or near 25 °C. Values for enthalpies and entropies of phase transitions are also included. The literature coverage is from 1881 through most of 1982 and there are detailed references given to the source literature.

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- [31] Domalski, E. S., W. H. Evans and T. L. Jobe, Jr., (principal contributors)  
Thermodynamic Data for Waste Incineration  
(The American Society of Mechanical Engineers, New York, 1979)

This 160 page monograph presents thermodynamic data for materials which are chemical mixtures, polymers, composite materials, solid wastes, and substances not easily identifiable by a single stoichiometric formula. The thermodynamic properties given are heats of reaction and transitions, heat capacities and heat contents, and vapor and sublimation pressures. Included is a material name and property index which covers approximately 600 materials, many of which are of biological interest, and including data on animals.

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- [32] Dorsey, N. E.  
Properties of Ordinary Water-Substance  
(Reinhold Publishing Corporation, New York, 1940)

This classic book is an exhaustive and critical compilation of the physical properties of water as reported in the literature through the year 1938. Essentially every physical property of pure water is covered. Although there is little emphasis on aqueous solutions, the solubilities and diffusion constants of selected gases in water are treated. Also see [134].

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- [33] Dymond, J. H. and Smith, E. B.  
The Virial Coefficients of Gases  
(Clarendon Press, Oxford, 1980)

This book is a critical compilation of the virial coefficients of about 300 gases at various temperatures. Included are references to the original sources as well as, in some cases, standard deviations and estimated inaccuracies for the data. This revised edition also includes data on gaseous mixtures.

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- [34] Fasman, G. D. (editor)  
Handbook of Biochemistry and Molecular Biology  
(CRC Press, Cleveland, Ohio, 1976)

This compilation is a revision and an expansion of the 1968 edition (see item [140]). Many of the earlier contributions have been revised. The three sections on the solubilities of fatty acids by K. S. Markley are in the

volume "Lipids, Carbohydrates, and Steroids" on pages 496 and 497. All of the other articles cited in item [140] appear in the volume "Physical and Chemical Reference Data" between pages 107 and 366. Items of interest which did not appear in the earlier edition are as follows:

<u>Author(s) or Source</u>	<u>Item</u>
E.D. Mooz	Data on the Naturally Occurring Amino Acids (Proteins, p. 111-174)

These tables include pK values for the amino acids at or near 25 °C.

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D. B. Dunn and R. H Hall	Purines, Pyrimidines, Nucleosides, and Nucleotides: Physical Constants and Spectral Properties (Nucleic Acids, p. 65-215)
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These tables include pK values for these materials at 25 °C.

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Interunion Commission on Biothermodynamics	Recommendations for Measurement and Presentation of Biochemical Equilibrium Data. (Physical and Chemical Reference Data, p. 93-103)
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This important report gives a set of recommendations pertinent to the measurement and treatment of biochemical equilibrium data.

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N. Langerman	Enthalpy, Entropy, and Free Energy Values for Biochemical Redox Reactions. (Physical and Chemical Reference Data, p. 121)
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This table summarizes  $\Delta G$ ,  $\Delta H$ , and  $\Delta S$  values for 14 biochemical redox reactions at 25 °C.

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- [35] Florkin, M. and Mason, H. (editors)  
Comparative Biochemistry, Volume II. Free Energy and Biological Function  
(Academic Press, New York and London, 1960)

This book contains several chapters dealing with the use of Gibbs energy data in biochemistry. The following chapters contain references to and/or tabulations of thermochemical data:

<u>Authors</u>	<u>Title of Chapter</u>
M. R. Atkinson and R. K. Morton,	Free Energy and Biosynthesis of Phosphates (Vol. 1, Chapter 1)



This chapter contains a tabulation of Gibbs energies and equilibrium constants for various metabolic processes involving phosphates. The temperature, pH, magnesium ion concentration, and appropriate literature references are given.

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L. F. Leloir, C. E. Cardini and E. Cabib      Utilization of Free Energy for the Biosynthesis of Saccharides (Volume 1, Chapter 2)

Included in the discussion are some references to equilibrium data relevant to the biosynthesis of saccharides.

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P. P. Cohen and G. W. Brown, Jr.      Ammonia Metabolism and Urea Biosynthesis (Volume 1, Chapter 4)

In their discussion of ammonia metabolism, the authors have used other compilations of thermodynamic data to compute Gibbs energy changes for these processes.

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[36] Fox, D., Labes, M. M. and Weissberger, A. (editors)  
Physics and Chemistry of the Organic Solid State  
(John Wiley and Sons, Interscience Publishers, New York 1963)

E. F. Westrum, Jr. and J. P. McCullough      Chapter 1. Thermodynamics of Crystals

In addition to discussion of thermodynamic properties of organic substances and their measurement, this chapter (178 pp.) gives tables of entropy of fusion, and vapor pressures and a table of thermodynamic data sources for about 800 organic compounds (798 references).

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[37] Franks, F. (editor)  
Water-A Comprehensive Treatise (in five volumes)  
(Plenum Press, New York and London, 1972 to 1975)

This treatise consists of forty-six chapters dealing with water and aqueous solutions. Although concerned with all aspects of water, several chapters contain extremely useful summaries of thermodynamic data. Among these are:

<u>Author(s)</u>	<u>Title of Chapter</u>
F. Franks	The Properties of Ice (Vol. 1, Chapter 4)

Tabulated are the ionic equilibrium constant and transport properties of ice at -10 °C.

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G. S. Kell

Thermodynamic and Transport Properties  
of Fluid Water (Vol. 1, Chapter 10)

Included is the density of water as a function of temperature, the vapor pressure, specific heat, partial molar volume, critical properties, and viscosity of water from 0 to 500 °C and to 8 kbar. Also see items [43] and [134].

K. Tödheide

Water at High Temperatures and Pressures  
(Vol. 1, Chapter 13)

This chapter is an extensive tabulation of the high temperature properties of water. Included are the specific volume, fugacity, Gibbs energy and enthalpy of formation, entropy, viscosity, thermal conductivity, dielectric constant, and ion product of water. The temperature and pressure ranges are 0 to 1000 °C and up to 250 kbar. Also see items [43] and [134].

F. Franks and D. S. Reid

Thermodynamic Properties  
(Vol. 2, Chapter 5)

Given are  $\Delta G^\circ$ ,  $\Delta H^\circ$ ,  $\Delta S^\circ$ , and  $\Delta C_p^\circ$  for the solution of hydrocarbons, alcohols, and rare gases in water at 25 °C.

H. L. Friedman and C. V. Krishnan

Thermodynamics of Ionic Hydration  
(Vol. 3, Chapter 1)

Tabulated are single-ion entropies of about 110 diatomic and polyatomic ions in water; Gibbs energies, enthalpies, and entropies of hydration of monatomic ions at 25 °C; partial molar volumes of about 120 common ions at 25 °C; ionic partial molar heat capacities of ions; Gibbs energies of transfer of inorganic electrolytes from H<sub>2</sub>O to D<sub>2</sub>O; and calorimetrically determined enthalpies of solution of salts in H<sub>2</sub>O and D<sub>2</sub>O.

D. Eagland

Nucleic Acids, Peptides, and Proteins  
(Vol. 4, Chapter 5)

Thermodynamic parameters for coil  $\rightarrow$  helix and homopolymer  $\rightarrow$  coil helix transitions of amino acids in aqueous solution are tabulated.

H. L. Anderson and R. H. Wood

Thermodynamics of Aqueous Mixed Electrolytes  
(Vol. 3, Chapter 2)

Included are data on the enthalpies and excess Gibbs energies of mixing of about 24 mixed electrolyte systems in water at 25 °C.

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- [38] Fredenslund, A., Gmehling, J. and Rasmussen, P.  
Vapor-liquid Equilibria Using UNIFAC  
(Elsevier Scientific Publishing Company, Amsterdam, 1977)

This book describes the UNIFAC (an acronym formed from Universal Quasi-Chemical Functional Group Activity Coefficient) procedure for estimating activity coefficients of non-electrolytes in fluid mixtures and the use of these activity coefficients for the prediction of vapor-liquid equilibria. The estimation scheme is based upon a group-contribution method. The methodology is clearly described with examples of its use and with computer programs listed in the Appendix to the volume. There is also a chapter which describes a procedure for estimating the second virial coefficients of gases. The coverage of materials and functional groups includes alcohols, alkanes, ethers, organic acids, ketones, aldehydes, amines, hydrocarbons, and nitrogen compounds.

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- [39] Freeman, R. D. (editor)  
Bulletin of Chemical Thermodynamics  
(Thermochemistry, Inc., Oklahoma State University, Stillwater, OK  
74078)

Each annual issues (volume 25 appeared in 1982) of the Bulletin is a current awareness index to, and a comprehensive bibliography of, articles that pertain to chemical thermodynamics (broadly interpreted) and that were published in the previous calendar year. The index is arranged by chemical substance and identifies the thermodynamic property reported for each substance; numerical data are not given. Four subdivisions of the index cover inorganic substances, organic substances, organic mixtures, and biochemical and macromolecular systems. Also included in each Bulletin is a section of Reports, on "work completed but not yet published", from a large number of laboratories located worldwide, a bibliography of recently published books related to thermodynamics, and a section of miscellaneous items of interest to the thermodynamic community. The early volumes of the "Annual Review of Physical Chemistry", published since 1950 by Annual Reviews, Inc., contained bibliographic information for general thermochemistry and the thermodynamics of electrolyte solutions; these articles were, in part, the forerunners of the Bulletin. From 1965 to 1976 the Bulletin had the title "Bulletin of Thermodynamics and Thermochemistry" and was published by the University of Michigan under the editorship of E.F. Westrum, Jr.

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- [40] Freir, R. K.  
Aqueous Solutions: Data for Inorganic Compounds (in two volumes)  
(Walter de Gruyter, Berlin and New York, 1976 and 1977)

This very well organized and easy-to-use handbook contains a wealth of thermodynamic data on aqueous solutions. There are 1300 solutions for which data is given. The solutes are both inorganic and organic, and include data on biochemical substances when available. Properties given are densities,

solubilities, equilibrium constants, Gibbs energies of formation, electrochemical potentials, conductivities, pH values, species-composition diagrams, and vapor pressures. The most serious shortcoming of this handbook is the absence of specific references to the literature sources of the data. The bulk of the text is in German.

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- [41] Goldberg, R. N., Staples, B. R., Nuttall, R. L. and Arbuckle, R. A Bibliography of Sources of Experimental Data Leading to Activity or Osmotic Coefficients for Polyvalent Electrolytes in Aqueous Solution (NBS Special Publication 485, U. S. Government Printing Office, Washington, D.C., 1977)

This is a bibliography of sources of experimental data that can be used to calculate either activity or osmotic coefficients of polyvalent electrolytes in water at the temperatures (0 to 100 °C) for which the data exist. The compounds are arranged according to the standard thermochemical order of arrangement. There are approximately 400 references to the source literature.

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- [42] Gurvich, L. V., Veits, I. V., Medvedev, V. A., Khachkuruzov, G.A., Yungman, V.S., Bergman, G.A. et al. "Termodinamicheskie Svoistva Individual'nykh Veshchestv" (Thermodynamic Properties of Individual Substances) V.P. Glushko, general editor Volume I, parts 1 and 2 (1978); Volume II, parts 1 and 2 (1979); Volume III, parts 1 and 2 (1981); Volume IV, in press. (Izdatel'stvo "Nauka", Moscow, 1979).

This extensive work is a critical evaluation and collection of the thermodynamic properties of the elements and their compounds. The properties tabulated are  $C_p^\circ$ ,  $(G^\circ - H^\circ(0))/T$ ,  $S^\circ$ , and  $H^\circ - H^\circ(0)$  and  $\log_{10}K$  where  $K$  for gases is the equilibrium constant for the reaction of forming the given compound from its atoms; for solids  $K$  refers either to vaporization or to atomization. The temperature range for which the data are given is 100 K to the highest temperature for which data exist, the temperature intervals being in steps of 100 K. There are extensive discussions of the sources from which the data have been taken, the computational procedures, and also, references to the source literature. Also see item [144]. The contents of the four volumes are:

<u>Volume</u>	<u>Contents</u>
I	O, H(D,T), F, Cl, Br, I, He, Ne, Ar, Kr, Xe, Rn, S, N, and P
II	C, Si, Ge, Sn, and Pb
III	B, H, Ga, In, Tl, Be, Mg, Ca, and Ba
IV	Cr, Mo, W, V, Nb, Ta, Ti, Zr, Hf, Sc, Y, La, Th, U, Pu, Li, Na, K, Rb, and Cs.

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- [43] Haar, L., Gallagher, J. S. and Kell, G. S.  
A Thermodynamic Surface for Water: The Formulation and Computer Programs  
(NBSIR 81-2253, National Bureau of Standards, Washington, D.C., 1981)

Haar, L., Gallagher, J. S. and Kell, G. S.  
The Anatomy of the Thermodynamic Surface of Water: The Formulation and  
Comparisons with Data  
(The American Society of Mechanical Engineers, New York, 1982)

Haar, L., Gallagher, J. S., and Kell, G. S.  
NBS-NRC Steam Tables  
(Hemisphere Press, Washington, DC, 1984)

The 1981 article summarizes the development of a thermodynamic surface for water with which all thermodynamic properties for the fluid states can be calculated from the freezing line to 1000 K and up to 1 GPa in pressure. The discussion is very brief, but gives references to earlier work and indicates that a more detailed publication is forthcoming. Given are coefficients of the Helmholtz function which define the surface. Plots of heat capacity, enthalpy, and speed of sound are included.

The 1982 report contains a computer program which can be used to calculate twelve thermodynamic properties of water and steam over the range  $0^{\circ}\text{C} \leq t \leq 1000^{\circ}\text{C}$  and  $0 \leq p \leq 1000\text{ MPa}$ . The properties include the Helmholtz function, the pressure, entropy, isochoric and isobaric heat capacity, the 2nd virial coefficient, and the speed of sound. Also see item [134].

The book in press contains tables, with documentation, for all of the equilibrium properties of water and steam for which reliable data exist. Also included in the book are tables of transport and mechanical property data such as the surface tension, the viscosity, and the thermal conductivity. The temperature range which the data tables extend is  $0^{\circ}\text{C} \leq t \leq 2500^{\circ}\text{C}$  and the pressure range is  $0 \leq p \leq 3000\text{ MPa}$ .

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- [44] Hala, E., Wichterle, I., Polak, J. and Boublík, T.  
Vapour-Liquid Equilibrium Data at Normal Pressures  
(Pergamon Press, Oxford, 1968)

This book contains correlated vapor-liquid-equilibrium data on mixtures (mostly binary but with some multicomponent systems). The correlations are done using any one of several approaches: The Antoine equation for a pure component, van Laar and Margules equations for mixtures. In all cases the source(s) of the experimental data is given. The coverage of systems (400) is very broad and it includes aqueous, nonaqueous, and organic-inorganic mixtures.

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- [45] Hamer, W. J. (editor)  
The Structure of Electrolytic Solutions  
(John Wiley and Sons, New York, 1959)

This book contains several chapters relevant to this bibliography. They are:

Author(s)

Title of Chapter

C. W. Davies

Incomplete Dissociation in Aqueous Salt Solutions (Chapter 3)

Tabulated are values of  $-\log_{10}K$  at 25 °C for the pairing in aqueous solution of eighteen common inorganic cations with thirty-eight of the more common inorganic and organic anions.

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E. Lange

Heats of Dilution of Dilute Solutions of Strong and Weak Electrolytes (Chapter 9)

This chapter contains a discussion of the theoretical interpretation and calculations of heats of dilution of electrolytes of various charge types with some information on non-electrolytes and weak electrolytes. Data from the literature are presented in graphical form. Included are data for eighteen inorganic electrolytes and seven inorganic non-electrolytes at 25 °C.

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H. S. Harned

Diffusion and Activity Coefficients of Strong and Weak Electrolytes (Chapter 10)

Tabulated are the activity coefficients, obtained from diffusion data, for twenty common aqueous electrolyte systems at 25 °C.

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F. H. Spedding and G. Atkinson

Properties of Rare Earth Salts in Electrolytic Solutions (Chapter 22)

Tabulated are the equivalent conductances, transference numbers, activity coefficients, densities and partial molar volumes, apparent molar compressibilities, heats of solution and dilution for the rare earth salts in aqueous solution at 25 °C.

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- [46] Hamer, W. J., and DeWane, H. J.  
Electrolytic Conductance and the Conductances of the Halogen Acids in Water  
(NSRDS-NBS 33, U. S. Government Printing Office, Washington, D.C., 1970)

This monograph contains a detailed evaluation of equivalent conductance data for hydrofluoric, hydrochloric, hydrobromic, and hydroiodic acids in water at various concentrations from -20 to +65 °C.

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- [47] Hamer, W. J. and Wu, Y. C.  
The Activity Coefficients of Hydrofluoric Acid in Water from 0 to 35 °C  
Journal of Research of the National Bureau of Standards 74A, 761 (1970)

This very detailed review on hydrofluoric acid contains critically evaluated data for the activity coefficient of HF as a function of molality and temperature (0 to 35 °C), equilibrium constants for the ionic association reactions characteristic of HF, calculated pH values, and calculated concentrations of the pertinent ions.

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- [48] Hamer, W. J. and Wu, Y. C.  
Osmotic Coefficients and Mean Activity Coefficients of Uni-Univalent Electrolytes in Water at 25 °C  
Journal of Physical and Chemical Reference Data 1, 1047 (1972)

This evaluation gives values for the osmotic coefficients and mean activity coefficients of seventy-nine uni-univalent electrolytes in aqueous solution at 25 °C, with values expressed on the molality scale. The data from the literature were fitted, by statistical procedures, to equations which express the quantities as functions of electrolyte concentration. Literature references are given to fifty-one additional uni-univalent electrolytes. Also see item [159].

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- [49] Harned, H. S. and Owen, B. B.  
The Physical Chemistry of Electrolytic Solutions (3rd Edition)  
(Reinhold Publishing Corporation, New York, 1958)

This book (about 800 pp.) is a treatise on the physical chemistry of electrolytic solutions with coverage of both equilibrium and non-equilibrium properties. The book includes tables of values of the equivalent conductance, dissociation constants, transference numbers, diffusion coefficients, relative apparent molar heat contents, activity coefficient, pH values, densities, and activity coefficients for many of the more common inorganic and organic electrolyte solutions.

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- [50] Harned, H. S. and Robinson, R. A.  
Multicomponent Electrolyte Solutions  
(Pergamon Press, Oxford, 1968)

This monograph deals with the theoretical and experimental aspects of multicomponent and largely inorganic electrolyte solutions, with emphasis upon the measurement and interpretation of activity coefficients, heats of mixing, and volume changes accompanying mixing. There is a useful bibliography of activity coefficient data for mixed electrolyte systems. We note, for the reader's information, the following monographs published in the same series of books (The International Encyclopedia of Physical Chemistry and Chemical Physics) and which deal principally with theory or methods of measurement pertinent to electrolyte solutions:

AuthorTitle of Volume

E. A. Guggenheim and R. H. Stokes

Equilibrium Properties of Aqueous  
Solutions of Single Strong Electrolytes

R. H. Stokes and R. Mills

Viscosity of Electrolytes and  
Related Properties

E. J. King

Acid-Base Equilibria

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- [51] Hawkins, D. T.  
Physical and Chemical Properties of Water:  
A Bibliography: 1957-1974  
(Plenum Press, New York, 1976)

This bibliography consists of 3600 references to the literature that deal with physical properties of pure water or dilute aqueous solutions. The papers are arranged by category of properties. Categories include thermodynamic properties, transport data, densities, acoustical, electrical, magnetic, and radiation properties. The bibliography covers the years 1957 to 1974. There is an author and keyword index. A bibliographic listing covering the years 1969 to 1974 appeared in the Journal of Solution Chemistry, 4, 621 (1976).

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- [52] Helgeson, H. C., Kirkham, D. H. and Flowers, G. C.  
Theoretical Prediction of the Thermodynamic Behavior of Aqueous  
Electrolytes at High Pressures and Temperatures: IV. Calculation  
of Activity Coefficients, Osmotic Coefficients, and Apparent  
Molal and Standard Relative Partial Molal Properties to 600 °C  
and 5 kb  
American Journal of Science 281, 1249 (1981)

This 268 page article is concerned with the prediction of the thermodynamic properties of aqueous electrolyte solutions at high temperatures and pressures. There is an extensive discussion of the fundamental thermodynamics of solutions and a discussion of theoretical concepts and models which have been used to describe electrolyte solutions. There is a very extensive bibliography ( 600 citations) which contains valuable references to specific systems of interest. Some specific tables of interest to this bibliography contain Debye-Hückel parameters at 25 °C, standard state partial molar entropies and heat capacities at 25 °C, and parameters for calculating activity coefficients, osmotic coefficients, relative apparent and partial molar enthalpies, heat capacities, and volumes at 25 °C.

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- [53] Hepler, L. G. and Hopkins, H. P., Jr.  
Thermodynamics of Ionization of Inorganic Acids and Bases in  
Aqueous Solution.  
Reviews in Inorganic Chemistry 1, 303 (1979)



The review contains a general discussion of the thermodynamics of aqueous acid-base chemistry. The systems which are discussed are pure water,  $\text{CO}_2 + \text{H}_2\text{O}$ ,  $\text{NH}_3 + \text{H}_2\text{O}$ , hydrofluoric acid, phosphoric acid, hydrogen sulfide,  $\text{SO}_2 + \text{H}_2\text{O}$ , sulfuric acid,  $\text{H}_2\text{CrO}_4$ ,  $\text{H}_2\text{Cr}_2\text{O}_7$ , iodic acid, and aqueous metal cations. This article cites values  $\Delta G^\circ$ ,  $\Delta H^\circ$ , and  $\Delta C_p^\circ$  for the ionizations of these various acids.

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- [54] Hepler, L. G. and others  
Thermochemistry of the Transition Metal Elements and Their Compounds

This series of papers contain critical reviews and selections of thermochemical data for the transition metal elements and their compounds. Tabulated are selected values of  $\Delta_f G^\circ$ ,  $\Delta_f H^\circ$ ,  $S^\circ$ , and electrode potentials at 25 °C. Each article contains a discussion of the data upon which the selections have been made and the references to the source literature. The papers in the series are:

Authors

Title of Paper

R. N. Goldberg and L. G. Hepler

Thermochemistry and Oxidation Potentials  
of the Platinum Group Metals and Their  
Compounds

Chemical Review 68, 229 (1968)

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L. M. Gedansky and L. G. Hepler

Thermochemistry of Silver and Its  
Compounds

Engelhard Industries Technical Bulletin IX, No. 4, 117 (1969)

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L. M. Gedansky and L. G. Hepler

Thermochemistry of Gold and Its Compounds

Englehard Industries Technical Bulletin X, No. 1, 5 (1969)

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L. M. Gedansky, E. M. Woolley and  
L. G. Hepler

Thermochemistry of Compounds and Aqueous  
Ions of Copper

Journal of Chemical Thermodynamics 2, 561 (1970)

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J. O. Hill, I. G. Worsley and  
L. G. Hepler

Thermochemistry and Oxidation Potentials  
of Vanadium, Niobium, and Tantalum

Chemical Reviews 71, 127 (1971)

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L. G. Hepler and G. Olofsson

Mercury: Thermodynamic Properties,  
Chemical Equilibria, and Standard  
Potentials

Chemical Reviews 75, 585 (1975)

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J. G. Travers, I. Dellien and  
L. G. Hepler

Scandium: Thermodynamic Properties,  
Chemical Equilibria, and Standard  
Potentials

Thermochimica Acta 15, 89 (1976)

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L. G. Hepler and P. P. Singh

Lanthanum: Thermodynamic Properties,  
Chemical Equilibria, and Standard  
Potentials

Thermochemica Acta 16, 95 (1976)

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I. Dellien, F. M. Hall and  
L. G. Hepler

Chromium, Molybdenum and Tungsten:  
Thermodynamic Properties, Chemical  
Equilibria, and Standard Potentials

Chemical Reviews 76, 283 (1976).

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T. A. Zordan and L. G. Hepler

Thermochemistry and Oxidation  
Potentials of Manganese and Its  
Compounds

Chemical Reviews 68, 737 (1968)

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- [55] Hirata, M., Ohe, S. and Nagakama, K.  
Computer Aided Data Books of Vapor-Liquid Equilibria  
(Kodansha Limited and Elsevier Scientific, Tokyo and New York, 1975)

This large volume (933 pages) contains tables, plots, and parameters pertinent to vapor-liquid-equilibria (VLE). VLE data for  $\approx 1000$  binary systems have been collected and treated by computer to obtain the tables and system graphs presented. References to the primary literature are included along with a detailed compound index. The coverage of compounds is very broad and includes a wide variety of organic mixtures and 30 organic-water mixtures.

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- [56] Horsley, L. H.  
 Azeotropic Data (in three volumes)  
 Advance in Chemistry Series No. 6, 35 and 116  
 (American Chemical Society, Washington, D.C., 1952, 1962 and 1973)

This series is concerned with the properties of azeotropic mixtures, specifically boiling temperatures, pressures, vapor-liquid equilibrium data, and compositions. Each of the volumes contains references to the source literature for each of the system catalogued. In terms of coverage of mixtures, the series is comprehensive for both binary and ternary mixtures and covers both inorganic and organic materials. The most recent volume contains a section dealing with the prediction and calculation of azeotropic mixtures.

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- [57] Horvath, A. L.  
 Reference Literature to the Critical Properties of Aqueous Electrolyte Solutions  
 Journal of Chemical Information and Computer Sciences 15, 245 (1975)

This bibliography gives references to the critical properties of aqueous electrolyte solutions. The bibliography covers  $\approx 75$  solutions and has 85 references.

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- [58] Horvath, A. L.  
 Reference Literature to Solubility Data between Halogenated Hydrocarbons and Water  
 Journal of Chemical Documentation 12, 163 (1972)

This is a bibliography giving 103 references to solubility data for halogenated hydrocarbons ( $C_1$  to  $C_6$ ) in water. References are given for approximately 100 compounds.

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- [59] Ingraham, L. L. and Pardee, A. B.  
 Free Energy and Entropy in Metabolism  
 in Metabolic Pathways, Volume I  
 (D. M. Greenberg, editor)  
 (Academic Press, New York, 1967)

This chapter contains a general discussion of the thermodynamics of metabolic processes, with the (unevaluated) data itself being presented in the course of the discussion. The emphasis is almost entirely upon Gibbs energy changes measured under physiological or near physiological conditions. There are 143 references to the primary literature.

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- [60] Izatt, R. M., Christensen, J. J. and Rytting, J. H.  
 Sites and Thermodynamic Quantities Associated with Proton and Metal  
 Ion Interaction with Ribonucleic Acid, Deoxyribonucleic Acid, and Their  
 Constituent Bases, Nucleosides, and Nucleotides  
 Chemical Reviews 71, 439 (1971)

This review contains twenty-three pages of tables of thermodynamic data ( $\log K$ ,  $\Delta H$ ,  $\Delta S$ , and  $\Delta C_p$ ) pertinent to the interaction of protons and metal ions with the nucleic acids and their molecular components together with the methods and experimental conditions (pH, temperature, ionic strength) used in their determination. There are 229 references.

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- [61] Janz, G. J.  
 Thermodynamic Properties of Organic Compounds  
 Estimation Methods, Principles, and Practice (revised edition)  
 (Academic Press, New York and London, 1967)

This well-established monograph discusses computation of thermodynamic properties such as heat capacities, entropies, enthalpies and Gibbs energies by statistical-mechanical methods, by methods of structural similarity, by methods of group contributions, by methods of group equations, and by methods of generalized vibrational assignments. The chemical properties: enthalpy of formation, and enthalpy of combustion are treated in terms of bond energies and group increments. Some 78 tables are given of increments, group contributions, and bond contributions as specifically needed for estimation of particular properties.

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- [62] Janz, G. J. and Tomkins, R. P. T.  
 Non-Aqueous Electrolytes Handbook (in two volumes)  
 (Academic Press, New York, 1972)

These volumes contain extensive tabulations of physical data pertinent to non-aqueous solvents, both single solvent and mixed solvent systems. The properties that are tabulated include melting point, boiling point, dielectric constant, viscosity, specific conductance, density, transference number, solubility, enthalpy of solution and dilution,  $E^\circ$  values for electrochemical cells, vapor pressure, polarographic data, ligand exchange rate, and spectroscopic data. The vast majority of the approximately 300 solvent systems dealt with are organic. There is a substance-property index, and sources of data are referenced.

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- [63] Jones, M. N. (editor)  
 Biochemical Thermodynamics  
 (Elsevier Scientific Publishing Co., Amsterdam, 1979)

This book is divided into eleven chapters, each on a topic pertinent to biochemical thermodynamics and written by an expert on that topic. Each chapter contains useful references to papers in the literature which contain tabular summaries of thermodynamic data pertinent to the theme of that chapter. The chapters and authors are:



<u>Author(s)</u>	<u>Title of Chapter</u>
M. N. Jones	The Scope of Thermodynamics in Biochemistry
F. Franks	Aqueous Solution Interactions of Low Molecular Weight Species - The Applicability of Model Studies in Biochemical Thermodynamics
W. Pfeil and P. L. Privalov	Conformational Changes in Proteins
H. J. Hinz	Conformation Changes in Nucleic Acids
D. S. Reid	Thermodynamics of Aqueous Polysaccharide Solutions
M. N. Jones	The Thermal Behavior of Lipid Systems and Biological Membranes
S. J. Gill	Ligand Binding of Gases of Hemoglobin
M. Monti and I. Wadsö	Calorimetric Studies in Blood Cells
G. C. Krescheck	Thermochemical Studies on Bacterial and Mammalian Cells
A. G. Lowe	Energetics of Muscular Contraction
B. Crabtree and D. J. Taylor	Thermodynamics and Metabolism

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- [64] Jordan, T. E.  
Vapor Pressure of Organic Compounds  
(John Wiley and Sons, Interscience Publishers, New York, 1954)

This is a comprehensive compilation (266 pages) of vapor pressure data for organic compounds. Included are tables on the hydrocarbons, alcohols, aldehydes, esters, ketones, acids, phenols, and metal organic compounds. Data for each compound are shown in graphical form, i.e. vapor pressure as a function of temperature. References to the data sources in the literature are given.

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- [65] Joshi, R. M. and Zwolinski, B. J.  
Heats of Polymerization and Their Structural and Mechanistic Implications  
in Vinyl Polymerization, Volume 1, Part I, edited by G. E. Ham  
(Marcel Dekker, New York, 1967)

The authors discuss experimental methods used to measure and derive enthalpies of polymerization. A listing of experimental data on enthalpies of polymerization is provided for 81 organic polymerization reactions. Other tables give enthalpies of formation, enthalpies of vaporization, entropies, Gibbs

energies, equilibrium constants, rate constants and activation energies at 25 °C for a variety of polymerization processes. A discussion of the structural influence upon the enthalpy of polymerization is also given. At the end of the chapter, 164 references are cited.

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- [66] Kaimakov, E. A. and Varshavskaya, N. L.  
Measurement of Transport Numbers in Aqueous Solutions of Electrolytes  
Russian Chemical Reviews (Uspekhi Khimii) 35, 89 (1966)

This review article summarizes the various methods available for the measurement of transference numbers. The authors have included a table which summarizes available (thru 1966) transport number data for aqueous electrolyte solutions, including references to the source literature.

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- [67] Karapet'yants, M. Kh. and Karapet'yants, M. L.  
Thermodynamic Constants of Inorganic and Organic Compounds  
(Ann Arbor Humphrey Science Publishers, Ann Arbor and London, 1970)  
Translated from the Russian:  
"Osnovnye Termodinamicheskie Konstanty Neorganicheskikh i Organicheskikh Veshchestv"  
(Izdatel'stvo "Khimiya", Moscow, 1968)

This book is a compilation of  $\Delta_f G^\circ$ ,  $\Delta H_f^\circ$ ,  $S^\circ$ , and  $C_p$  values at 298.15 K for about 4000 substances in the condensed and gaseous phases, and in aqueous solution. Covered are not only the inorganic elements and their compounds, but also data for the organic compounds through 34 carbon atoms. The authors point out that their tabulated values do not always form a self-consistent system of thermodynamic data. There are 2733 references.

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- [68] Kaufmann, D. W. (editor)  
Sodium Chloride  
(Reinhold Publishing Corporation, New York, 1960)

This monograph, published under the auspices of the American Chemical Society, has in its Appendix a useful compilation of the physical properties of aqueous sodium chloride solutions. Included are essentially all of the measured equilibrium and transport properties of this system at various temperatures and pressures. The data are well referenced.

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- [69] Kazavchinskii, Ya. Z., Kessel'man, P. M., Kirillin, V. A.,  
Riukin, S., Sheindlin, A. E., Shpil'rain, E. E., Sychev, V. V. and  
Timrot, D. L. (edited by V. A. Kirillin)  
Heavy Water-Thermophysical Properties  
(U. S. Department of Commerce, National Technical Information Service,  
Springfield, VA 1971)  
Translated from the Russian:  
"Tyazelaya voda. Teplofizicheskie Svoistva"  
(Gosudarstvennoe energeticheskoe izdatel'stvo, Moskva-Leningrad, 1963)

This treatise is an exhaustive compilation of physical data on heavy water (deuterium oxide). Some of the more relevant properties that are covered include densities, critical constants, vapor pressures, enthalpies of transition, viscosity, and thermal conductivity, equation of state, and tables of thermodynamic properties as functions of temperature and pressure.

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- [70] Keenan, H. J., Keyes, G. F., Hill, P. G. and Moore, J. G.  
Steam Tables - Thermodynamic Properties of Water, Including Vapor, Liquid, and Solid Phases (International Edition, Metric Units)  
(John Wiley and Sons, New York, 1969)

This book presents the results of a reassessment and correlation of the thermodynamic data for water. It supersedes the Keenan and Keyes Tables of 1936. Values are tabulated for the specific volume, internal energy, and enthalpy, as functions of temperature and pressure. Also given are data for vapor-liquid and vapor-solid equilibrium, superheated vapor, and the compressed liquid. Mollier and temperature-entropy charts are included along with charts of heat capacity of liquid and vapor, Prandtl number, and isentropic expansion coefficient. The data and tables are discussed in an appendix of 25 pages and a list of 37 references is given. Also see items [43] and [134] for other correlations.

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- [71] Kertes, A. S. (editor-in-chief)  
Solubility Data Series  
(Pergamon Press, New York, 1979 to 1981)

This eighteen volume series, prepared under the auspices of the IUPAC, is a part of a continuing project concerned with the preparation of a comprehensive, critical compilation of data on solubilities in all physical systems including gases, solids, and liquids. The volumes which have been issued to date, with their titles and editors, are:

<u>Editor(s)</u>	<u>Title</u>	<u>Volume Numbers</u>
H. L. Clever	Helium and Neon - Gas Solubilities	1
H. L. Clever	Krypton, Xenon, and Radon - Gas Solubilities	2
M. Salomon	Silver Azide, Cyanide, Cyanamides, Cyanate Selenocyanate and Thiocyanate	3
H. L. Clever	Argon	4
C. L. Young	Hydrogen and Deuterium	5/6
R. Battino	Oxygen and Ozone	7
C. L. Young	Oxides of Nitrogen	8
W. Hayduk	Ethane	9
R. Battino	Nitrogen and Air	10
B. Scrostai and C. A. Vincent	Alkali Metal and Alkaline-Earth Metal and Ammonium Halides. Amide Solvents	11
O. Popovych	Tetraphenylborates	18

The following volumes are planned for future publication:

Z. Galus and C. Guminski	Metals in Mercury	12
C. L. Young	Oxides of Nitrogen, Sulfur and Chlorine	13
R. Battino	Nitrogen	14
H. L. Clever and W. Gerrard	Hydrogen Halides in Non-Aqueous Solvents	15
A. L. Horvath	Halogenated Benzenes	16
E. Wilhelm and C. L. Young	Hydrogen, Deuterium, Fluorine and Chlorine	17

In general, for each system covered in this series, the preparer, who is identified, gives the following information: the components in the system, the intensive variables, the experimental values of the solubility, the experimental methodology and source and purity of materials, a discussion of the evaluation procedure, estimates of error, and literature citations.

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- [72] Kirgintsev, A. N., Trushnikova, L. N., and Lavrenteva, V. F.  
Solubilities of Inorganic Substances in Water  
(in Russian)  
(Izdatelstvo Khimiya, Leningrad, 1972)

This book consists of aqueous phase diagrams of pure salts in water. The phase diagrams cover the composition and temperature ranges for which the data exist. The diagrams are particularly useful in assessing the regions of stability of the various inorganic hydrates and in obtaining solubilities. The authors have included references to the source literature from which the data have been obtained. The coverage of inorganic salts spans the periodic chart. There are data for  $\approx 1200$  inorganic salts which are indexed in the Appendix to the book.

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- [73] Kortum, G., Vogel, W. and Andrussov, K.  
Dissociation Constants of Organic Acids in Aqueous Solution  
(Butterworths, London, 1961)

This book is a compilation of 1056 dissociation constants of organic acids in aqueous solution, presented in tabular form. Introductory and explanatory remarks are in both German and English. Remarks in the Table are in German. Part I is a critical discussion of techniques for measurements of dissociation constants by conductance, electrometric, catalytic and optical methods. Each method is classified and assigned a code in Part II, which deals with use of the tables, and methods of calculation. The Tables themselves are arranged by acid class including: aliphatic and alicyclic carboxylic acids, aromatic carboxylic acids, phenolic acids, and other acids and special classes. The Tables contain the name, chemical formula, and thermodynamic dissociation constant  $K$  of each acid, the temperature ( $^{\circ}\text{C}$ ) of measurement, the range of concentration over which the measurements were made, code for the method of measurement, calculation procedure and any corrections made, a critical evaluation of the quality of the measurement, and the source reference. All



data were drawn from the literature, covering the period between 1927 and 1956, and are referenced in a classified reference list. A compound index is provided.

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- [74] Kragten, J.  
Atlas of Metal-Ligand Equilibria in Aqueous Solution  
(Ellis Horwood, Chichester, England, 1978)

This book contains  $\approx 750$  pages of predominance, or species-composition diagrams, for aqueous solutions involving 45 metals and 25 common ligands. Most of the thermodynamic data was taken from Sillen and Martell and from Smith and Martell (see items [89] and [137]).

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- [75] Krebs, H. A. and Kornberg, H. L., with appendix by K. Burton  
Energy Transformations in Living Matter  
(Springer-Verlag, Berlin, 1957)

The main part of this monograph surveys the various biochemical pathways by which living systems utilize energy. In the Appendix are (1) Tables of Gibbs energies of formation of ninety-eight compounds of biological importance, (2) Gibbs energies and electrochemical potentials of important biological oxidation-reduction reactions, and (3) Gibbs energy changes accompanying the processes of glycolysis and alcoholic fermentation, the tricarboxylic acid cycle, and hydrolysis. The source of data is given for each entry.

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- [76] Landolt-Börnstein  
Numerical Data and Functional Relationships in Science and Technology

Several volumes in the Landolt-Börnstein series contain data relevant to this bibliography. They are:

<u>Author(s)</u>	<u>Title of Volume</u>	<u>Location</u>
G. Beggerow	Heats of Mixing and Solution	New Series, Group IV, Volume 2

This very extensive volume (695 pages) contains data on heats of mixing, solution, and dilution for both organic and inorganic substances. The coverage of substances spans the periodic chart and includes both binary and multi-component mixtures. The data on each system include the components of the mixture, the temperature, the composition, the enthalpies, and the appropriate literature citations.

(K.-H. Hellwege, editor, Springer-Verlag, Berlin, 1976)

J. D'Ans, H. Surawski      Densities of Binary, Aqueous      New Series, Group IV,  
and C. Synowietz      Systems and Heat Capacities      Volume 1  
of Liquid Systems

This 123 page section contains extensive tables of the specific heats of binary, and a few ternary, aqueous systems at the temperatures and molalities for which data exist. The authors include plots of the data and references to the source literature.

(K.-H. Hellwege, editor, Springer-Verlag, Berlin, 1977)

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W. Auer, H. D. Baer,      Kalorische Zustandsgrößen      6th Edition, Volume 2,  
K. Bratzler, F. Burhorn,      Part 4  
H. Kientz, O. Kubachevski,  
Fr. Losch, A. Neckel, H.  
Nelkanski, Kl. Schäffer,  
and R. Wienecke

This volume contains thermal properties: molar heat capacity, entropy, enthalpy, enthalpy of formation, Gibbs energy of formation, in the standard state, and enthalpies of phase changes for many organic and inorganic substances in SI units. The dependence of thermal functions and heat capacity upon temperature is given for many substances. Some other thermodynamic quantities are given. Extensive tables are given of group contributions to enthalpies of formation and the Gibbs energies of formation of organic substances (gases) in  $\text{kcal}\cdot\text{mol}^{-1}$  and  $\text{kJ}\cdot\text{mol}^{-1}$ . Many of the heat capacity data are presented in diagrams. This series also includes tables of freezing point depressions, conductivities, transference numbers, and densities for aqueous systems.

(K. Schäfer and E. Lax, editors, Springer-Verlag, Berlin, 1961)

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J. Weishaupt      Thermodynamic Equilibria of      New Series, Group IV,  
Boiling Mixtures      Volume 3

This volume deals with the thermodynamic vapor-liquid equilibrium of binary and multicomponent mixtures. The coverage of systems extends across the periodic chart. The mixtures are adequately indexed and the reference to the primary literature given. The information given on a typical system includes tables of equilibrium temperatures as a function of the mole fractions of the components at a given pressure with accompanying figures.

(H. Hausen, editor, Springer-Verlag, Berlin, 1976)

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- [77] J. A. Larkin (editor)  
International Data Series B. Thermodynamic Properties of Aqueous Organic Systems  
(Engineering Sciences Data Unit, London, 1978 and 1979)

This part of the International Data Series deals with the thermodynamic properties of approximately 100 aqueous organic systems. Tabulated are excess properties (G, H, C, and V), vapor-liquid equilibrium data, and vapor pressures as a function of composition. Each table is prepared by an individual contributor and includes, in a very neat tabular form, the tables of property values, the correlating equations and their coefficients, the methods of measurement, a brief discussion, and the appropriate references to the literature.

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- [78] Latimer, W. M.  
The Oxidation States of the Elements and Their Potentials in Aqueous Solution  
(second edition)  
(Prentice-Hall, Englewood Cliffs, New Jersey, 1959)

This book contains extensive tables of  $\Delta_f G^\circ$ ,  $\Delta_f H^\circ$ ,  $S^\circ$  values for the elements and their compounds as well as electrode potential diagrams calculated from the tabulated  $\Delta_f G^\circ$  values, from other measurements, and estimates when appropriate. Many of the tabulated data were taken from National Bureau of Standards Circular 500 (see item [131]). The appendices include activity coefficient data for 77 strong electrolytes and a discussion of methods whereby entropies may be estimated.

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- [79] Lewis, G. N. and Randall, M.  
(revised by K. S. Pitzer and L. Brewer)  
Thermodynamics  
(McGraw-Hill, New York, 1961)

This standard textbook on chemical thermodynamics contains an Appendix (no. 4) of selected data for aqueous electrolyte solutions. Compiled are activity coefficients, Debye-Hückel parameters, relative partial molar enthalpies, and relative partial molar heat capacities for about 70 of the most common electrolytes in aqueous solution at 25 °C. More recent Debye-Hückel parameters are to be found in the pages of Pitzer, Peiper, and Busey and of Bradley and Pitzer (see item [121]) and the paper of Clarke and Glew, item [22].

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- [80] Leyendekkers, J. V.  
Thermodynamics of Seawater  
(Marcel Dekker, New York and Basel, 1976)

This book deals with the thermodynamic properties of seawater as a multicomponent electrolyte solution. Each chapter covers a thermodynamic property of seawater and its constituents. There are chapters on the fundamentals of thermodynamics, the entropy, the volume, the expansibility, and the compressibility. Included in each chapter is a discussion of the methods for calculating or estimating the desired property with tables of values of experimental and calculated properties. There are extensive references to the primary

literature. The author has indicated that a second volume was to be published, but it has not yet appeared in print. Also see [126].

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- [81] Linke, W. F.  
Solubilities: Inorganic and Metal-Organic Compounds--A Compilation of Solubility Data from the Periodical Literature. Volume I: A-Ir, Volume II: K-Z  
(Volume I: D. Van Nostrand Co., Princeton, New Jersey, 1958 )  
(Volume II: American Chemical Society, Washington, D.C., 1965)

These two volumes (total of 3401 pages) are comprehensive compilations of mostly unevaluated solubility data for inorganic and metal-inorganic compounds. Both aqueous and non-aqueous solvent systems are included. The temperatures and compositions given cover the ranges for which experimental data exist. References are given to the data sources. These two volumes had their origins in the solubility compilations begun by A. Seidell in 1907.

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- [82] Lobo, V. M. M.  
Electrolyte Solutions: Literature Data on Thermodynamic and Transport Properties  
(Coimbra Editora, Coimbra, Portugal, 1975)

This monograph is a compilation of physical property data on aqueous salt solutions. The properties tabulated are the density, the conductance, transference number, viscosity, diffusion coefficient and the activity coefficient. The monograph contains data on approximately 70 binary systems at temperatures and compositions for which experimental data exist and includes an index and references to the sources of the data.

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- [83] Long, C. (editor)  
Biochemists Handbook  
(D. Van Nostrand Co., Princeton, New Jersey, 1961)

This reference book contains several tables of thermochemical data:

<u>Author(s)</u>	<u>Title of Section</u>
S. P. Datta and A. K. Grzybowski	pH and Acid-Base Equilibria (pages 19 to 58)

This section contains a discussion of pH scales and the electrometric measurement of pH, tables of assigned pH values for various buffered solutions, and tables (about 600 entries) of thermodynamic acid dissociation constants of weak organic acids (some as a function of temperature).



K. Burton

Free Energy Data and Oxidation-  
Reduction Potentials  
(pages 93 to 95)

This section contains some revisions and additions to Burton's earlier tables (see, in this bibliography, the book by Krebs and Kornberg, item [75]).

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- [84] Long, F. A. and McDevit, W. F.  
Activity Coefficients of Non-electrolyte Solutes in Aqueous Salt Solutions  
Chemical Reviews 51, 119 (1952)

This review article is concerned with the effect of salts on the activity coefficients of non-electrolytes. There is an extensive discussion of both the theoretical and experimental procedures used in the study of this phenomena. There is an extensive appendix to the article which lists salt effects on non-polar electrolytes ( $\approx 100$  systems). The article has 180 references.

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- [85] MacKay, D. and Shiu, W. Y.  
A Critical Review of Henry's Law Constants for Chemicals of Environmental Interest  
Journal of Physical and Chemical Reference Data 10, 1175 (1981)

This is a critical review and tabulation of Henry's Law constants, vapor pressures, and solubilities in water of 150 organic substances of environmental importance. The compounds include gaseous, liquid, and solid alkanes, cycloalkanes, alkenes, alkynes, monoaromatics, polynuclear aromatics, halogenated alkanes, alkenes and aromatics, and selected pesticides. Nearly all of the data refer to 25 °C.

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- [86] Maczynski, A., Maczynska, Z., Rogalski, M., Skrzecz, A., and Dunajska, K.  
Verified Vapor-Liquid Equilibrium Data (in four volumes)  
(PWN - Polish Scientific Publishers, Warsaw, 1976 to 1979)

This four volumes series contains vapor-liquid equilibrium data (i.e., compositions of vapor and liquid phases as functions of temperature and pressure) covering the regions for which experimental measurements exist. The systems are almost entirely organic. The data have been recalculated into SI units and have been smoothed in many cases, often using the Redlich-Kister equation. There are detailed references to the source literature and there is an alphabetic index of the systems covered. The four volumes are:

Author(s)Title

A. Maczynski	Binary Hydrocarbon Systems
A. Maczynski, Z. Maczynska, and M. Rogalski	Binary Systems of Hydrocarbons and Related Non-Oxygen Compounds
A. Maczynski, Z. Maczynska, and A. Skrzecz	Binary Systems of Organic Compounds Containing Halogen, Nitrogen and Sulfur
A. Maczynski, Z. Maczynska, T. Treszczanowicz, and K. Dunajska	Binary Systems of Hydrocarbons and Oxygen Compounds Without Alcohols and Acids

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- [87] Marcus, Y., Kertes, A. and Yanir, E.  
Equilibrium Constants of Liquid-Liquid Distribution Reactions (in three  
volumes)  
(Butterworths, London, 1974 and 1977)

This three volume series contains equilibrium data on liquid-liquid distribution reactions. The equilibria of concern include: distribution, dissociation and aggregation of the extractant, reactions of the extractant with diluents and with other solvents, extraction of the water, equilibria of the extraction metal ions, and extraction of metal ions with the extractant as the ligand. Volumes 1 and 2 cover organophosphorous extractions and alkylammonium salt extractants, respectively. Volume 3 deals with distribution reactions of carboxylic and sulfonic acid extractants, and the distribution of inorganic acids, salts, and complexes between aqueous solutions and both inert solvents and solvents which have oxygen donor atoms. Each reaction entry includes the equilibrium constant, the temperature for which the data exists, the conditions, and a reference(s) to the source literature.

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- [88] Marshall, W. L. and Franck, E. U.  
Ion Product of Water Substance, 0-1000 °C, 1-10,000 bars  
New International Formulation and its Background  
Journal of Physical and Chemical Reference Data 10, 295 (1981)

The ion-product of water is represented as a function of temperature (0 to 1000 °C) and pressure (1 to 10,000 bars) by an equation with adjustable parameters which have been determined by least-squares procedures using data from the literature. The paper also contains the background for the international formulation for the ion-product of water as issued by the International Association for the Properties of Steam in May 1980. Also see [108].

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- [89] Martell, A. E. and Smith, R. M.  
Critical Stability Constants. Volume 1: Amino Acids  
(Plenum Press, New York, 1974)
- Smith, R. M. and Martell, A. E.  
Critical Stability Constants. Volume 2: Amines  
(Plenum Press, New York, 1975)
- Martell, A. E. and Smith, R. M.  
Critical Stability Constants. Volume 3: Other Organic Ligands  
(Plenum Press, New York, 1977)
- Smith, R. M. and Martell, A. E.  
Critical Stability Constants. Volume 4: Inorganic Complexes  
(Plenum Press, New York, 1976)

and

- Martell, A. E. and Smith, R. M.  
Critical Stability Constants. Volume 5: First Supplement  
(Plenum Press, New York, 1982)

Volume 1 contains selected values of  $\log K$ ,  $\Delta H$ , and  $\Delta S$  at 25 °C for the interaction of inorganic metal and hydrogen ions with several classes of organic ligands. The organic ligands dealt with are the aminocarboxylic acids, iminodiacetic acid and its derivatives, peptides, aniline carboxylic acids, pyridine carboxylic acids, peptides, and several other miscellaneous ligands. The data are critically selected from the literature rather than being simply compiled. Each selected datum contains a reference to the primary literature. This 469 page volume contains a ligand formula and name index.

Volume 2 is similar in arrangement to Volume 1. The organic ligands dealt with are the aliphatic, secondary, and tertiary amines, azoles, azines, and the amino phosphorous acids.

Volume 3 contains the organic ligands which are not contained in Volumes 1 and 2. These ligands include carboxylic and phosphorous acids, phenols, alcohols, amides, amines, halides, and many others.

Volume 4 is similar in arrangement to the earlier volumes. The ligands dealt with are the hydroxide ion, some of the transition metal ligands (vanadium, chromium, molybdenum, tungsten, and others) and ligands of the Groups III through VII elements.

Volume 5 is a supplement to the first four volumes and serves to make the coverage of the literature more current. Also see item [137].

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- [90] McGlashan, M. L. (editor)  
Chemical Thermodynamics (in two volumes)  
(The Chemical Society, London, 1971 and 1978)

This two volume series contains reviews of the current literature pertinent to several specialized areas of chemical thermodynamics. Each chapter is written by a specialist in that area and includes many useful references to the primary literature. The chapters and their authors are:

<u>Volume 1</u>	<u>Title of Chapter</u>
M. L. McGlashan	The Scope of Chemical Thermodynamics
E.F.G. Herrington	Thermodynamic Quantities, Thermodynamic Data, and their Uses
A. J. Head	Combustion and Reaction Calorimetry
J. F. Martin	The Heat Capacities of Organic Compounds
J.D. Cox and I. W. Lawrenson	The p, V, T Behavior of Single Gases
J. F. Counsell	Modern Vapourflow Calorimetry
D. Ambrose	Vapour Pressures
S. G. Frankiss and J. H. S. Green	Statistical Methods for Calculating Thermodynamic Functions
O. Kubaschewski, P. J. Spencer and W. A. Dench	Metallurgical Thermochemistry at High Temperatures

<u>Volume 2</u>	
K. N. Marsh	The Measurment of Thermodynamic Excess Functions of Binary Liquid Mixtures
T. M. Letcher	Activity Coefficients at Infinite Dilution from Gas-Liquid Chromatography
C. L. Young	Experimental Methods for Studying Phase Behavior of Mixtures at High Temperatures and Pressures
G. M. Schneider	High-Pressure Phase Diagrams and Critical Properties of Fluid Mixtures
F. L. Swinton	Mixtures Containing a Fluorocarbon
A. G. Williamson	Specific Interactions in Nonelectrolyte Mixtures
C. M. Knobler	Volumetric Properties of Gaseous Mixtures
R. L. Scott	Critical Exponents for Binary Fluid Mixtures
C. P. Hicks	A Bibliography of Thermodynamic Quantities for Binary Fluid Mixtures

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- [91] McMeekin, T. L.  
The Solubility of Biological Compounds  
in "Solutions and Solubilities," Part I. (M. R. J. Dack, editor)  
(John Wiley and Sons, New York, 1975)

This chapter contains a discussion on systematic studies on the solubilities of proteins and lipids. The author has attempted to relate solubility to structure and has included several tables and plots giving solubilities of amino acids, proteins, lipids and fatty acids. There are 62 references to the literature.

\* \* \* \* \*

- [92] McMillen, D. F. and Golden, D. M.  
Hydrocarbon Bond Dissociation Energies  
Annual Reviews of Physical Chemistry 33, 493 (1982)

This review article contains "best" values of bond-dissociation energies at 298.15 K of hydrocarbons and their nitrogen, oxygen, sulfur, halogen, and silicon derivatives. There is also some limited data on inorganic molecules. The tables include data on  $\Delta_f H^\circ$  of the related radicals. The authors provide references to a dozen earlier reviews on this subject and there are 242 references to the source literature. Also see item [162].

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- [93] Medvedev, V. A., Bergman, G. A., Gurvich, L. V., Yungman, V. S., Vorob'ev, A. F., Kolesov, V. P. and others (V. P. Glushko, general editor)  
Thermal Constants of Substances (Volumes 1 to 10)  
(in Russian)  
(Viniti, Moscow, 1965 to 1982)

This extensive series represents many years of effort by numerous Russian thermodynamicists engaged in the critical evaluation of thermodynamic data. Included in the tables are carefully selected values of  $\Delta_f G^\circ$ ,  $\Delta_f H^\circ$ ,  $S^\circ$ ,  $H_T - H_0$ , and  $C_p$  at 298.15 K for the elements and their compounds including many aqueous species. Also given are dissociation energies of gases and enthalpies of phase changes. There are extensive references to the primary literature from which the tabulated values were obtained. Carbon and its compounds are covered up to two carbon atoms. The coverage and arrangements of substances is similar to that used in the NBS Tables of Chemical Thermodynamic Properties (see item [149]).

\* \* \* \* \*

- [94] Meites, L. (editor)  
Handbook of Analytical Chemistry  
(McGraw-Hill Book Co., New York, 1963)

This treatise on analytical chemistry contains several useful tabulations of thermochemical data. Some of these tabulations are taken directly from other sources cited in this bibliography and are not included below:

Author(s)Title of Section

V. E. Bowers and R. G. Bates

Equilibrium Constants of Proton-transfer  
Reactions in Water  
(Section 1, Table 1-10)

Tabulated are pK values at 15, 25, and 35 °C for about 200 organic and inorganic acids; no literature references are given.

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L. Meites
Formal Equilibrium Constants of Proton-  
transfer Reactions at Finite Ionic Strength  
(Section 1, Table 1-11)

This section contains a tabulation of pK values at 25 °C for a selected series of about 150 acids, and bases. These data were taken from Bjerrum, Schwarzenbach, and Sillen, "Stability Constants of Metal Complexes," Part I, The Chemical Society, London, 1957 which was later revised by Sillen and Martell (see item [137]). Also given are tables of acid dissociation data pertinent to ethanol-water and methanol-water mixtures.

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D. A. Aikens and C. N. Reilley
Formation Constants of Metal Complexes  
(Section 1, Table 1-17)

Tabulated are log K values for the binding of the more common inorganic metal ions to 55 ligands.  $\Delta H$  and  $\Delta S$  values are also given for four ligands. Literature references are given.

\* \* \* \* \*

- [95] Merrill, A. L. and Watt, B. K.  
Energy Value of Foods: Basis and Derivation  
Agriculture Handbook No. 74  
(U.S. Government Printing Office, Washington, D.C., 1955)

Watt, B. K. and Merrill, A. L.  
Composition of Foods: Raw, Processed, Prepared  
Agriculture Handbook No. 8 (revised)  
(U. S. Government Printing Office, Washington, D.C., 1963)

This pair of monographs provides numerous composition and energy values for food and foodstuff ingredients. It should be noted, of course, that the Calorie used in food energy values is one kilocalorie (4.184 kJ) as used in thermochemistry. In Agriculture Handbook No. 74, Part I gives a discussion of the sources of food energy in terms of organic compound class, and of the experimental determination of enthalpies of combustion. Parts II, III, and IV apply the data to physiological processes. An appendix gives composition and enthalpy of combustion of foods. Tables 1 to 5 and table 24 give enthalpies of combustion of specific food items or component substances. Care should be used in taking values from the numerous tables, as correction factors have

sometimes been applied to adjust for physiological processes. These adjustments are indicated by footnotes. In Agriculture Handbook No. 8, Appendix A is of particular interest as it gives notes on energy values and nutrients, including (adjusted) enthalpies of combustion of many foods and food ingredients.

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- [96] Milazzo, G. and Caroli, S.  
Tables of Standard Electrode Potentials  
(John Wiley and Sons, New York, 1978)

This book contains extensive tables of standard electrode potentials covering the periodic chart. For each electrode reaction is given the standard potential, the temperature and the pressure, the solvent, and a literature reference. Occasionally the temperature coefficient of the electrode potential is given together with an estimate of uncertainty. Much of the tabulated data is taken from secondary sources (such as item [149]).

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- [97] Miller, D. G.  
Application of Irreversible Thermodynamics to Electrolyte Solutions.  
I. Determination of Ionic Transport Coefficients  $\ell_{ij}$  for Isothermal Vector Transport Processes in Binary Electrolyte Systems.  
Journal of Physical Chemistry 70, 2639 (1966)  
II. Ionic Coefficients  $\ell_{ij}$  for Isothermal Vector Transport Processes in Ternary Systems.

These papers derive equations relating fundamental isothermal transport coefficients ( $\ell_{ij}$ 's) to experimentally measurable quantities for electrolytes in a neutral solvent.  $\ell_{ij}$ 's for the most common aqueous ionic solutions are calculated from critically reviewed data.

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- [98] Millero, F. J.  
The Partial Molal Volumes of Electrolytes in Aqueous Solutions.  
Compilation of the Partial Molal Volumes of Electrolytes at Infinite Dilution,  $V^\circ$  and the Apparent Molal Volume Concentration Dependence Constants,  $S^*$  and  $b_\gamma$ , at Various Temperatures, in  
Water and Aqueous Solutions, R. A. Horne (editor)  
(John Wiley and Sons, Interscience Publishers, New York, 1972)

This chapter (no. 13 in this book) is concerned with the measurement and interpretation of partial molar volumes and their concentration and temperature dependence. Included are tables of the partial molar volumes of the common inorganic and organic electrolytes (about 200 systems) as well as values of the partial molar volumes of the more common inorganic and organic ions (about 100 species). The data refer to temperatures from 0 to 200 °C. Also see items [99] and [123].

\* \* \* \* \*

- [99] Millero, F. J.  
The Molal Volumes of Electrolytes  
Chemical Reviews 71, 147 (1971)

This is a detailed and thorough review article dealing with molar volumes of electrolytes in water. Included is a history and discussion of theoretical developments associated with molar volumes. Tabulated are the partial molar volumes of the common (about 50) inorganic and organic ions in water at temperatures ranging from zero to 200 °C. Also is given partial molar volume data for non-aqueous systems. There are 366 references to the literature. Also see item [98] and [123].

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- [100] Mishchenko, K. P. and Poltoratzkii, G. M.  
Aspects of the Thermodynamics and Structure of Aqueous and Non-Aqueous  
Electrolyte Solutions  
(in Russian)  
(Izdatelstvo Khimia, Leningrad, 1968)

This 350 page monograph contains extensive discussions and correlations (theoretical and empirical) of existing experimental data on enthalpies, Gibbs energies, and entropies, of solution and ionization of inorganic acids, bases, and salts in water and selected organic solvents. Heat capacities, enthalpies, Gibbs energies, and entropies of the substances and their ions in solution are also discussed. Extensive use is made of diagrams relating observed properties to periodic groupings of the elements. The monograph contains numerous small tables of properties of limited groups of substances. A summary compilation of selected values of thermodynamic properties occupies 43 pages, giving  $\Delta_f G^\circ$ ,  $\Delta_f H^\circ$ ,  $S^\circ$  and  $C_p^\circ$  of pure and dissolved inorganic substances in their standard state at 25 °C, selected enthalpies of solution at 25 °C, enthalpies of dilution of common acids, bases, and salts at 25 °C, and heat contents and partial molar heat capacities for selected salts vs. concentration and temperature in water, methanol, ethanol, and a few other organic solvents.

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- [101] Morss, L. R. Thermochemical Properties of Yttrium, Lanthanum,  
and the Lanthanide Elements and Ions  
Chemical Reviews 76, 827 (1976)

This review presents tables of values of  $\Delta_f H^\circ$ , and  $S^\circ$  at 25 °C for the aqueous ions of yttrium, lanthanum, and the lanthanide elements based upon both experimental measurement data and a group correlation scheme.

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- [102] Nancollas, George H.  
Interactions in Electrolyte Solutions  
(Elsevier, Amsterdam, 1966)

This monograph contains a general discussion of the methodology, kinetics, mechanisms, structural features, and general thermodynamic trends of ionic association reactions in solution. In the Appendix there are several tables of thermodynamic functions for ion-association reactions with references to the source literature.

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- [103] Naumov, G. B., Rhyzhenko, B. N. and Khodakovsky, I. L.  
Handbook of Thermodynamic Quantities  
(in Russian)  
(Atomizdat, Moscow, 1971)

This reference book contains a compilation of thermodynamic data for about 2000 chemical compounds and aqueous ions (mostly inorganic). The thermodynamic properties tabulated are  $\Delta_f G^\circ$ ,  $\Delta_f H^\circ$ ,  $S^\circ$ , and  $C_p^\circ$  at 298.15 K, electrode potentials, enthalpies and entropies for phase transitions,  $\Delta_f G^\circ$  of inorganic aqueous ions from 25 to 350 °C, partial molar heat capacities from 10 to 130 °C, and the partial molar volumes of aqueous electrolytes at high temperatures and pressures. There are 1550 references given to the primary literature and to the literature evaluations of others.

\* \* \* \* \*

- [104] National Bureau of Standards Electrolyte Data Center  
A series of papers, published in the Journal of Physical and Chemical Reference Data from 1977 to 1981.

This series of papers contains evaluations leading to recommended values of activity and osmotic coefficients and excess Gibbs energies of aqueous electrolyte solutions at 298.15 K. The data are presented both in tabular form as a function of molality and as coefficients of several correlating equations. The correlations are detailed and include a careful statistical analysis of the data and references to the source literature. The data cover the entire composition range for which data exist and include most of the electrolytes of charge type 12 and 21 (also see items [48], [121], [124], and [128]). The papers in the series are:

<u>Author(s)</u>	<u>Title of Paper</u>
B. R. Staples and R. L. Nuttall	The Activity and Osmotic Coefficients of Aqueous Calcium Chloride at 298.15 K
Journal Physical and Chemical Reference Data <u>6</u> , 385 (1977)	
R. N. Goldberg and R. L. Nuttall	Evaluated Activity and Osmotic Coefficients for Aqueous Solutions: The Alkaline Earth Metal Halides
Journal of Physical and Chemical Reference Data <u>7</u> , 263 (1978)	
R. N. Goldberg, B. R. Staples and R. L. Nuttall	Evaluated Activity and Osmotic Coefficients for Aqueous Solutions: Iron Chloride and the Bi-univalent Compounds of Nickel and Cobalt

Journal of Physical and Chemical Reference Data 8, 923 (1979)

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R. N. Goldberg

Evaluated Activity and Osmotic Coefficients for  
Aqueous Solutions: Bi-univalent Compounds of  
Lead, Copper, Manganese, and Uranium

Journal of Physical and Chemical Reference Data 8, 1005 (1979)

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R. N. Goldberg

Evaluated Activity and Osmotic Coefficients for  
Aqueous Solutions: Bi-univalent Compounds of  
Zinc, Cadmium, and Ethylene Bis  
(Trimethylammonium) Chloride and Iodide

Journal of Physical and Chemical Reference Data 10, 1 (1981).

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R. N. Goldberg

Evaluated Activity and Osmotic Coefficients for  
Aqueous Solutions: Thirty-Six Uni-Bivalent  
Electrolytes

Journal of Physical and Chemical Reference Data 10, 761 (1981)

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B. R. Staples

Activity and Osmotic Coefficients of Aqueous  
Metal Nitrites

Journal of Physical and Chemical Reference Data 10, 765 (1981)

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B. R. Staples

Activity and Osmotic Coefficients of Aqueous  
Sulfuric Acid

Journal of Physical and Chemical Reference Data 10, 779 (1981)

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[105] Nývlt, J. Solid-Liquid Phase Equilibria (Elsevier, Amsterdam, 1977)

This 246 page monograph contains tables of solubilities as a function of temperature of approximately 350 compounds to form binary and ternary mixtures. The substances are mostly inorganic and include only 22 organic compounds. Also included are enthalpies of solution of the substances into pure water. The author does not give references to the primary literature.

\* \* \* \* \*

- [106] Oetting, F.L., Medvedev, V., Rand, M.H. and Westrum, E.F., Jr. (editors)  
The Chemical Thermodynamics of Actinide Elements and Compounds  
(International Atomic Energy Agency, Vienna, 1976 to present)

This series of books contains thermodynamic data (heat capacities, formation properties, thermal functions, vapor pressures, and many other properties) for the actinide elements and their compounds. In addition to extensive tables of data there is also a discussion of the sources from which the data have been taken and the calculations performed. Parts 2 and 3 contain data on the aqueous ions of the actinide elements. To date, the parts which have been published are:

<u>Author(s)</u>	<u>Title</u>	<u>Part No.</u>
F.L. Oetting, M.H. Rand and R. J. Ackermann	The Actinide Elements	1
J. Fuger and F. L. Oetting	The Actinide Aqueous Ions	2
E. H. P. Cordfunke and P. A. G. O'Hare	Miscellaneous Actinide Compounds	3
P. Chioti, V. V. Akhachinskij, I. Ansara, and M. H. Rand	The Actinide Binary Alloys	5

Parts 4 (Chalcogenides), 6 (Carbides), 7 (Pnictides), and 8 (Halides) are scheduled for publication in 1983.

\* \* \* \* \*

- [107] Ohe, S. (editor)  
Computer Aided Data Book of Vapor Pressure  
(Data Book Publishing Co., Tokyo, 1976)

This lengthy book (2000 pages) contains extensive plots of vapor pressures for various pure substances, both organic and inorganic, as a function of temperature as well as the constants of the Antoine equation. Included is a substance index and references to the literature.

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- [108] Olofsson, G. and Hepler, L. G.  
Thermodynamics of Ionization of Water Over Wide Ranges of Temperature and Pressure  
Journal of Solution Chemistry 4, 127 (1975)

This review ties together equilibrium and thermal data to obtain "best" values for  $\Delta G^\circ$ ,  $\Delta H^\circ$ ,  $\Delta C_p^\circ$ ,  $\Delta V^\circ$ , and  $\Delta \kappa^\circ$  (the isothermal compressibility change) for the ionization of water over the temperature range 0 to 300 °C and the pressure range 1 to 8000 atmospheres. Also see item [88].

\* \* \* \* \*

- [109] Parker, V. B., Staples, B. R., Jobe, T. L., Jr. and Neumann, D. B. A  
Report on Some Thermodynamic Data for Desulfurization Processes  
(NBSIR 81-2345, National Bureau of Standards, Washington, D.C., 1981)

This report contains values of thermochemical properties and processes pertinent to coal gas desulfurization. Substances covered include solutions formed from the aqueous ions;  $\text{OH}^-$ ,  $\text{SO}_3^{2-}$ ,  $\text{HSO}_3^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{CO}_3^{2-}$ ,  $\text{HCO}_3^-$ ,  $\text{H}^+$ ,  $\text{Mn}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Ca}^{2+}$ ,  $\text{Na}^+$ , and  $\text{K}^+$  and include solid, liquid, aqueous and gaseous compounds or species formed from these ions. Properties given are  $\Delta_f G^\circ$ ,  $\Delta_f H^\circ$ ,  $S^\circ$ ,  $C_p^\circ$ ,  $(H_T - H_0)$ ,  $L_\phi$ ,  $\gamma_\pm$ , and  $\phi$  at 298.15 K. Predicted values of  $\Delta_f G^\circ$ ,  $\Delta_f H^\circ$ ,  $\Delta S^\circ$ , and  $\Delta C_p^\circ$  for important desulfurization processes were calculated from the formation properties. These data are consistent with the data in item [149].

\* \* \* \* \*

- [110] Parker, V. B.  
The Thermochemical Properties of the Uranium-Halogen Containing Compounds  
(NBSIR 80-2029, National Bureau of Standards, Washington, D.C., 1980)

This report contains a detailed evaluation of the thermochemistry of 142 uranium-halogen containing compounds. The properties given are  $\Delta_f H^\circ$ ,  $\Delta_f G^\circ$ ,  $S^\circ$ ,  $C_p^\circ$ , and  $(H_T - H_0)$ , all at 298.15 K, and  $\Delta_f H^\circ$  at 0 K. The analysis of much of the data involves the consideration of the aqueous chemistry of uranium containing compounds (also see item [149]). The recommended values are consistent with the CODATA scale (item [23]).

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- [111] Parker, V. B.  
Thermal Properties of Aqueous Uni-univalent Electrolytes  
(NSRDS NBS 2, U.S. Government Printing Office, Washington, D.C., 1965)

This monograph is a review of the heat-capacity, enthalpy-of-solution, and enthalpy-of-dilution data on simple 1-1 electrolytes, organic and inorganic, in aqueous solutions. From the critical analysis of this data, tables of selected "best" values of apparent heat capacities, and enthalpies of dilution are given, as well as selected values of the enthalpies of solution to the infinitely dilute solution. Also included is a review of data on the enthalpies of neutralization of monobasic acids which has led to a selected "best" value for the enthalpy of ionization of water. Data on each property are introduced with a discussion of methods employed in reducing the data to a standard form and are listed by compound, in the order: acids, ammonium and amine salts, silver salts, and salts of the alkali metals. For each compound are listed the various investigations, with the temperature and range of concentrations measured. Graphs of molar heat capacity and molar enthalpy as functions of concentration are also included, for aqueous solutions of many of the compounds discussed. In addition, there is an abbreviated listing, by compound, of review and compilation papers on the thermal properties of the aqueous uni-univalent electrolytes. These and other references are also listed alphabetically in a separate reference section with 652 entries. The chosen "best" values at 25 °C for each parameter and compound are arranged in a series of 21 tables.

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- [112] Parker, V.B., Wagman, D. D. and Garvin, D.  
Selected Thermochemical Data Compatible with the CODATA Recommendations  
(NBSIR 75-968, National Bureau of Standards, Washington, D.C., 1976)

Selected thermochemical properties,  $\Delta_f G^\circ$ ,  $\Delta_f H^\circ$ ,  $S^\circ$ , (all at 298.15 K),  $\Delta_f H^\circ$  (0 K), and  $H$  (298.15 K) -  $H$  (0 K), are given for 384 substances (almost entirely inorganic) including many of the more commonly encountered aqueous species. The selected values are intended to be compatible with the current CODATA recommendations on key values for thermodynamics (see item [23]).

\* \* \* \* \*

- [113] Parsons, R.  
Handbook of Electrochemical Constants  
(Academic Press, New York, 1959)

This handbook contains extensive tables of data for the more common inorganic and organic aqueous electrolyte solutions. Properties covered include dielectric constants, activity coefficients, relative partial molar enthalpies, equilibrium constants, solubility products, conductivities, electrochemical potentials, Gibbs energies and enthalpies of formation, entropies, heat capacities, viscosities, and diffusion coefficients. Unfortunately, only a few of the tables contain references to the sources of the data.

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- [114] Pauling, L.  
The Nature of the Chemical Bond (third edition)  
(Cornell University Press, Ithaca, New York, 1960)

This well established monograph provides general information about the nature of chemical bonding in (principally) inorganic compounds which is fundamentally very important for the estimation of enthalpies of formation, but not always easily applied.

\* \* \* \* \*

- [115] Pedley, J. B. (editor)  
Computer Analysis of Thermochemical Data (CATCH Tables)  
(University of Sussex, Brighton, England, 1972 to 1974)

These thermochemical tables consist of enthalpies of formation at 298.15 K calculated from thermochemical data networks. Included are appropriate references to the literature and estimated errors in the enthalpies of formation. An interesting and important feature of this scheme is that the tables can be readily updated by computer. These tables contain a substantial amount of data for aqueous species. The following tables have been published:

<u>Author(s)</u>	<u>Element(s)</u>	<u>Year</u>
J. D. Cox	Halogen Compounds (Fluorine, Chlorine, Bromine, Iodine)	1972

G. Pilcher	Nitrogen	1972
A. J. Head	Phosphorus	1972
J. B. Pedley and B. S. Iseard	Silicon	1972
D. S. Barnes	Chromium, Molybdenum and Tungsten	1974

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- [116] Pedley, J. B. and Rylance, J.  
Sussex - N. P. L. Computer Analysed Thermochemical Data:  
Organic and Organometallic Compounds  
(Sussex University, Brighton, England, 1977)

This book contains enthalpy data on  $\approx 4000$  compounds and 5000 chemical processes involving organic and organometallic compounds. Much of the processing of the data was done by computer (see item [150]). Properties which are presented include enthalpies of combustion, formation, sublimation, vaporization, and reaction. It is also a revision of the values published by Cox and Pilcher (item [28]). There are  $\approx 450$  references to the sources from which the data were taken.

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- [117] Perrin, D. D.  
Dissociation Constants of Inorganic Acids and Bases in Aqueous Solution  
(Butterworths, London, 1969)

This short (163 pp.) monograph is a compilation of dissociation constants of 217 inorganic acids and bases. The classes of compounds include not only conventional acids and bases, but also hydrated metal ions and free radicals, such as hydroxyl, the only criterion being gain or loss of a proton or hydroxyl ion. The data are organized into a single table listing the compounds, preceded by a brief introduction to the use of table, and a section on methods of measurement and calculation. The methods are classified as conductometric, electrometric, optical, or other. Elements and compounds are listed in decreasing extent of protonation.  $pK$  values are, wherever possible, obtained by extrapolation to zero ionic strength. The table also gives the temperature of each measurement, remarks as to ionic strength, concentration, and any other factors relating to  $pK$ , coded references to method of measurement, the procedure used in evaluating the constants and any corrections taken into consideration, and the literature references. There are approximately 1100 references listed alphabetically by author.

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- [118] Perrin, D. D.  
Dissociation Constants of Organic Bases in Aqueous Solution  
(Butterworths, London, 1965)

This book contains values of dissociation constants for organic bases in aqueous solution. The bases are arranged under the headings aliphatic, alicyclic, aromatic, heterocyclic, natural products, dyes and indicators, substances lacking a basic nitrogen atom, and miscellaneous. Accompanying the data entry for each base is the temperature, method of measurement, formula, assessment of the measurement, and the appropriate reference. There are 3790 data entries in this book. Also see item [73].

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- [119] Phillips, R.  
Adenosine and the Adenine Nucleotides. Ionization, Metal Complex Formation, and Conformation in Solution  
Chemical Reviews 66, 501 (1966)

This article is a detailed review of the thermodynamics, kinetics, and structural characteristics of adenosine and the adenine nucleotides in solution. Both log K and enthalpy data are tabulated for protonation and metal-ion binding reactions to adenosine and the adenine nucleotides. The conditions are given under which the tabulated data are applicable, namely, ionic strength, temperature, supporting electrolyte, pH, method of measurement, as well as references to the original data source.

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- [120] Phillips, R. C., George, P., and Rutman, R. J.  
Thermodynamic Data for the Hydrolysis of Adenosine Triphosphate as a Function of pH,  $Mg^{2+}$  Ion Concentration, and Ionic Strength  
Journal of Biological Chemistry 244, 3330 (1969)

This article deals with the computation of the Gibbs energy change for the hydrolysis of adenosine-5'-triphosphate to adenosine-5'-diphosphate as a function of magnesium ion concentration, pH, and ionic strength at 25 °C. A critical evaluation of the existing data pertinent to this computation is included. References to 24 papers are given. Also see item [1].

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- [121] Pitzer, K. S. and others  
Thermodynamics of Electrolytes  
(A series of papers published in several journals)

This series of papers contains an extensive array of correlated data on aqueous electrolyte solutions, much of it having been calculated using the system of equations given in paper I in this series. The contents of these papers have been summarized by Pitzer in a chapter in the book edited by Pytkowicz (see item [123]). The data include activity and osmotic coefficients, relative apparent molar enthalpies and heat capacities, excess Gibbs energies, entropies, heat capacities, volumes, and some equilibrium constants and enthalpies. Systems of interest include both binary solutions and multi-component mixtures. While most of the data pertain to 25 °C, the papers on sodium chloride, calcium chloride, and sodium carbonate cover the data at the temperatures for which experiments have been performed. Also see items [48], [104], and [124].

The papers in this series which contain data relevant to this bibliography are:

Pitzer, K.S.

Thermodynamic Properties of Aqueous Solutions of Bivalent Sulphates  
Journal of the Chemical Society, Faraday Transactions II 68, 101 (1972).

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Pitzer, K.S. and Mayorga, G.

Thermodynamics of Electrolytes. II. Activity and Osmotic Coefficients for Strong Electrolytes with One or Both Ions Univalent  
Journal of Physical Chemistry 77, 2300 (1973).

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Pitzer, K.S. and Mayorga, G.

Thermodynamics of Electrolytes. III. Activity and Osmotic Coefficients for 22 Electrolytes  
Journal of Solution Chemistry 3, 539 (1974).

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Pitzer, K.S. and Kim, J.J.

Thermodynamics of Electrolytes IV. Activity and Osmotic Coefficients for Mixed Electrolytes  
Journal of the American Chemical Society 96, 5701 (1974).

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Pitzer, K.S. and Silvester, L.F.

Thermodynamics of Electrolytes. VI. Weak Electrolytes Including  $H_3PO_4$   
Journal of Solution Chemistry 5, 269 (1976).

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Pitzer, K.S., Roy, R.N. and Silvester, L.F.

Thermodynamics of Electrolytes VII. Sulfuric Acid  
Journal of the American Chemical Society 99, 4930 (1977).

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Silvester, L.F. and Pitzer, K.S.

Thermodynamics of Electrolytes. 8. High-Temperature Properties, Including Enthalpy and Heat Capacity, with Application to Sodium Chloride  
Journal of Physical Chemistry 81, 1822 (1977).

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Pitzer, K.S., Peterson, J.R. and Silvester, L.F.

Thermodynamics of Electrolytes. IX. Rare Earth Chlorides, Nitrates and Perchlorates.  
Journal of Solution Chemistry 7, 45 (1978).

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Silvester, L.F. and Pitzer, K.S.  
Thermodynamics of Electrolytes. X. Enthalpy and the Effect of Temperature  
on the Activity Coefficients.  
Journal of Solution Chemistry 7, 327 (1978).

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Pitzer, K.S. and Silvester, L.F.  
Thermodynamics of Electrolytes. II. Properties of 3:2, 4:2, and Other  
High-Valence Types  
Journal of Physical Chemistry 82, 1239 (1978).

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Bradley, D.J. and Pitzer, K.S.  
Thermodynamics of Electrolytes 12. Dielectric Properties of Water and Debye-  
Hückel Parameters to 350 °C and 1 kbar  
Journal of Physical Chemistry 83, 1599 (1979).

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Pitzer, K.S. and Peiper, J.C.  
Activity Coefficients of Aqueous  $\text{NaHCO}_3$ .  
Journal of Physical Chemistry 84, 2396 (1980).

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Peiper, J.C. and Pitzer, K.S.  
Thermodynamics of Aqueous Carbonate Solutions Including Mixtures of  
Sodium Carbonate, Bicarbonate, and Chloride  
Journal of Chemical Thermodynamics 14, 613 (1982).

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Rogers, P.S.Z. and Pitzer, K.S.  
Volumetric Properties of Aqueous Sodium Chloride Solutions  
Journal of Physical and Chemical Reference Data 11, 15 (1982).

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Pitzer, K.S.  
Theory: Ion Interaction Approach in "Activity Coefficients in Electrolyte  
Solutions," R.M. Pytkowicz (editor)  
(CRC press, Boca Raton, Florida, 1979).

See item [123]

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Roy, R.N., Gibbons, J.J., Peiper, J.C. and Pitzer, K.S.  
Thermodynamics of the Unsymmetrical Mixed Electrolyte  $\text{HCl-LaCl}_3$   
Journal of Physical Chemistry, 87, 2365 (1983).

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deLima, M.C.P and Pitzer, K.S.  
 Thermodynamics of Saturated Aqueous Solutions Including Mixtures of  
 NaCl, KCl, and CsCl  
 Journal of Solution Chemistry, 12, 171 (1983).

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deLima, M.C.P. and Pitzer, K.S.  
 Thermodynamics of Saturated Electrolyte Mixtures of NaCl with Na<sub>2</sub>SO<sub>4</sub>  
 and with MgCl<sub>2</sub>  
 Journal of Solution Chemistry, 12, 187 (1983).

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Phutela, R.C. and Pitzer, K.S.  
 Thermodynamics of Aqueous Calcium Chloride  
 Journal of Solution Chemistry, 12, 201 (1983).

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Pitzer, K.S., Peiper, J.C. and Busey, R.H.  
 Thermodynamic Properties of Aqueous Sodium Chloride Solutions  
 Journal of Physical and Chemical Reference Data, in review

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[122] Pourbaix, M. (and others)  
 Atlas of Electrochemical Equilibrium in Aqueous Solution  
 (Pergamon Press, Oxford, 1966)

This book contains tabulations of Gibbs energy of formation data for many of the principal compounds of the inorganic elements. Electrochemical potentials and their dependence on pH, are calculated for many important couples. Much of the Gibbs energy data is taken from the evaluations and compilations of others. Of particular utility are the species-composition or predominance diagrams which appear in this book.

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[123] Pytkowicz, R. M. (editor) Activity Coefficients in Electrolyte Solutions  
 (in two volumes) (CRC Press, Boca Raton, Florida, 1979)

This two volume series has several chapters dealing with various aspects of electrolyte solutions. The chapters which contain tables of thermodynamic data and/or a particularly useful collection of references to such literature are:

<u>Author</u>	<u>Title of Chapter</u>
K. S. Pitzer	Theory: Ion Interaction Approach

This chapter (no. 7 in Volume I) contains a summary of much of the research done by K. S. Pitzer and his collaborators on the development

of models for electrolyte solutions and on the representation of thermodynamic properties of electrolyte solutions in terms of these models. The tables in this chapter include: Debye-Hückel parameters for the osmotic coefficient, enthalpy, and heat capacity as a function of temperature; parameters for the activity and osmotic coefficients of approximately 270 aqueous strong electrolytes at 25 °C; parameters for the relative apparent molar and excess enthalpy of  $\approx 90$  strong electrolytes at 25 °C; a table of parameters for the activity and osmotic coefficients of  $\approx 75$  binary mixtures with and without common ions and with up to three solutes present; and parameters for the thermodynamic properties of aqueous NaCl and  $\text{H}_2\text{SO}_4$  as a function of temperature. The author has included references to his earlier papers which also contain valuable data on electrolyte solutions (also see item [121]).

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F. J. Millero

Effects of Pressure and Temperature on  
Activity Coefficients

This very extensive (99 pages) chapter (no. 2 in Volume II) contains a general discussion of the effects of temperature and pressure on activity coefficients for both binary and mixed electrolyte solutions. Properties of interest are the partial molar volume, expansibility, compressibility, heat capacity, and enthalpy. There is also an excellent discussion of methods of estimating partial molar properties in mixed electrolyte solutions. There are 226 references to the literature. Tables of data are presented for: Debye-Hückel limiting law slopes for the apparent molar volume, enthalpy, heat capacity, expansibility, and compressibility as a function of temperature; parameters for the partial molar volumes of 30 aqueous electrolytes at 25 °C; parameters for the partial molar expansibility of ten electrolytes at 25 °C; parameters for the partial molar compressibilities of 33 electrolytes at 25 °C; values of the activity coefficients of aqueous NaCl solutions at 25 °C as a function of pressure (up to 1000 bars); parameters for the partial molar enthalpies of 59 electrolytes at 25 °C; parameters for the partial molar heat capacities of 140 electrolytes at 25 °C; and tables giving compositions and the partial molar properties of average seawater.

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M. Whitfield

Activity Coefficients in Natural Waters

This long (147 pages and 266 references) and very detailed chapter (no. 3 in Volume II) contains a very extended discussion of the thermodynamics of mixtures of aqueous electrolyte solutions with emphasis upon the properties of natural waters. There is a very extensive collection of tables in this article (116 in total) and the contents of this many tables is not easily summarized in our survey. Included are the following: association constants for the formation of ion pairs and weak acids; activity coefficients for both the ions and major components of sea water; formation constants for the binding of heavy metals to several anions found in sea water; gas solubilities including carbon dioxide in sea water; solubilities of polychlorinated biphenyls in sea water;

Setchenow coefficients for hydrocarbons and for volatile solutes in sea water; the osmotic coefficient and density of sea water as a function of temperature and salinity. Thermodynamic solubility products of minerals in brines; the activity coefficient of carbon dioxide in sea water; speciation calculations on copper, zinc, cadmium, and lead in sea water; excess Gibbs energies of mixing of electrolyte solutions at 25 °C; and pairwise and triplet interaction terms for electrolyte solutions in terms of various models.

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- [124] Rard, J. A., Habenschuss, A. and Spedding, F. H.  
 A Review of the Osmotic Coefficients of Aqueous  $H_2SO_4$  at 25 °C  
 Journal of Chemical and Engineering Data 21, 374 (1976)  
 and  
 A Review of the Osmotic Coefficients of Aqueous  $CaCl_2$  at 25 °C  
 Journal of Chemical and Engineering Data 22, 180 (1977)

These two articles are critical evaluations of experimental data leading to values of the osmotic coefficients at 25 °C of the two reference electrolytes calcium chloride and sulfuric acid. Also see items [104] and [121].

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- [125] Reid, R. C., Prausnitz, J. M., and Sherwood, T. K.  
 The Properties of Gases and Liquids, Their Estimation and Correlation  
 (third edition)  
 (McGraw-Hill, New York, 1977)

This lengthy monograph discusses various methods available for calculation of estimating properties of materials, and then provides recommendations for action with respect to each kind of property. Included in the book are procedures for making estimates of critical constants, normal boiling temperatures, Lennard-Jones potential parameters, compressibility factors and equations of state, liquid molar volumes and densities, and vapor pressures. Estimates of enthalpies of vaporization, of ideal-gas heat capacities, and of enthalpies and Gibbs energies of formation are treated. For real fluids variations of enthalpy, entropy, internal energy, and heat capacity with pressure are treated. Some methods are given for estimating the properties of fluid mixtures. Surface tension and the transport properties-viscosity, diffusion coefficient and thermal conductivity-are discussed. Numerous tables present comparisons of observed and calculated properties. The Appendix contains tables of thermodynamic properties of many organic compounds.

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- [126] Riley, J. P. and Skirrow, G. (editors)  
 Chemical Oceanography (in six volumes)  
 (Academic Press, New York and London, 1975 and 1976)

This six volume series contains 34 chapters on various topics related to chemical oceanography. Contained in these chapters is a wealth of chemical and physical information on the properties of sea water and its constituents



as well as useful references to the primary literature. Several topics of thermodynamic interest are the solubilities of gases and salts, chemical speciation of the major and minor constituents of sea water, densities, activity and osmotic coefficients, expansibilities, isothermal compressibilities, velocity of sound, heat capacities, and transport and optical properties of sea water. The Appendix contains a useful series of tables of many of these properties. Also see [80].

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[127] Geological Survey Bulletins

Robie, R. A., Hemingway, B. S. and Fisher, J. R.  
Thermodynamic Properties of Minerals and Related Substances at 298.15 K  
and 1 Bar ( $10^5$  Pascals) Pressure and at Higher Temperatures  
Geological Survey Bulletin 1452  
(U.S. Government Printing Office, Washington, D.C., 1978)

and

Hemingway, B. S., Haas, J. L., Jr., and Robinson, G. R., Jr.  
Thermodynamic Properties of Selected Minerals in the System  
 $\text{Al}_2\text{O}_3$ -CaO-SiO<sub>2</sub>-H<sub>2</sub>O at 298.15 K and 1 Bar ( $10^5$  Pascals)  
Pressure and at Higher Temperature  
Geological Survey Bulletin 1544  
(U.S. Government Printing Office, Washington, D.C., 1982)

The 1978 publication is a 456 page monograph containing selected values for the entropy, molar volume, and for the enthalpy and Gibbs energy of formation for the elements, 133 oxides, and 212 other minerals and related substances at 298.15 K. Thermal functions are also given for those substances for which heat-capacity or heat-content data are available. The thermal functions are tabulated at 100 K intervals for temperatures up to 1800 K. The monograph includes detailed references to the source literature and a compound index. Also see items [42] and [144].

The 1982 publication is a supplement to Geological Survey Bulletin 1452. It contains a survey of thermodynamic data for minerals in the system  $\text{Al}_2\text{O}_3$ -CaO-SiO<sub>2</sub>-H<sub>2</sub>O and tabulated values for  $C^\circ$ ,  $(H^\circ - H^\circ(298.15 \text{ K}))/T$ ,  $(G^\circ - H^\circ(298.15 \text{ K}))/T$ ,  $\Delta_f H^\circ$ , and  $\Delta_f G^\circ$  from 298.15 to 1800 K. The calculations are well documented both as to computational procedures and the sources of data.

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- [128] Robinson, R. A. and Stokes, R. H.  
Electrolyte Solutions. The Measurement and Interpretation of  
Conductance,  
Chemical Potential and Diffusion in Solution of Simple Electrolytes  
(Second edition)  
(Butterworths, London, 1965)

In this, the revised second edition of a monograph first published in 1955, the first part presents a fundamental discussion of aqueous organic and inorganic electrolyte solutions. Included is a discussion of ionizing solvents (i.e. water), electrolytic conductivities and transport numbers, the

measurement and interpretation of chemical potentials; the theory of diffusion (emphasizing conductance and viscosity in concentrated solutions), and methods of measurement of diffusion coefficients. The final third of the text deals primarily with characteristics of specific electrolyte solutions, including weak and mixed electrolytes, and strong acids, and includes an extensive (98 pp.) appendix with approximately 75 tables of osmotic and activity coefficients, standard cell potentials ( $E^\circ$ ) in various organic solvents, ionic radii, and ionization constants of organic acids in aqueous solution, and other information. The narrative is supplemented with graphs, tables, equations, and references.

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- [129] Rosenblatt, David H. (editor)  
 Research and Development of Methods for Estimating Physicochemical  
 Properties of Organic Compounds of Environmental Concern (in two volumes)  
 (Arthur D. Little, Cambridge, Massachusetts, 1981)

These two volumes contain twenty-six chapters, each one dealing with a method for estimating a physico-chemical property of environmentally important organic compounds. For the most part, each chapter provides: "(1) a general discussion of the property and its importance in environmental considerations, (2) an overview of available estimation methods, (3) a description plus step-by-step instructions for each selected method, (4) worked-out examples for each method, (5) a listing of sources of available data on the property, (6) a list of symbols used, and (7) the cited references." The chapters in the book are:

<u>Author(s)</u>	<u>Title of Chapter</u>
W.J. Lyman	Octanol/Water Partition Coefficient
W.J. Lyman	Solubility in Water
W.J. Lyman	Solubility in Various Solvents
W.J. Lyman	Adsorption Coefficient for Soils and Sediments
S.E. Bysshe	Bio-concentration Factor in Aquatic Organisms
J.C. Harris and M.J. Hayes	Acid Dissociation Constant
J.C. Harris	Rate of Hydrolysis
J.C. Harris	Rate of Aqueous Photolysis
K.M. Scow	Rate of Biodegradation
W.J. Lyman	Atmospheric Residence Time
C. F. Grain	Activity Coefficient
C.E. Rechsteiner, Jr.	Boiling Point

C.E. Rechsteiner, Jr.	Heat of Vaporization
C.F. Grain	Vapor Pressure
R.G. Thomas	Volatilization from Water
R.G. Thomas	Volatilization from Soil
W.A. Tucker and L.H. Nelken	Diffusion Coefficients in Air and Water
J.H. Hagopian	Flash Points of Pure Substances
L.H. Nelken	Densities of Vapors, Liquids and Solids
C.F. Grain	Surface Tension
C.F. Grain	Interfacial Tension with Water
C.F. Grain	Liquid Viscosity
J.D. Birkett	Heat Capacity
J.D. Birkett	Thermal Conductivity
L.H. Nelken and J.D. Birkett	Dipole Moment
L.H. Nelken	Index of Refraction

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[130] Rossini, F. D., Pitzer, K. S., Taylor, W. J., Ebert, J. P.  
 Kilpatrick, J. E., Beckett, C. W., Williams, M. D. and Werner, H. C.  
 Selected Values of Properties of Hydrocarbons  
 National Bureau of Standards Circular C461  
 (U. S. Government Printing Office, Washington, D.C. 1947)

and

Rossini, F. D., Pitzer, K. S., Arnett, R. L., Brown, R. M. and  
 Pimentel, G. C.  
 Selected Values of Physical and Thermodynamic Properties of Hydrocarbons  
 and Related Compounds  
 (Carnegie Press, Pittsburgh, Pennsylvania, 1953)

This monograph resulted from the work of American Petroleum Institute (API) Research Project 44. In the 1953 revision, values are given for 40-odd physical and thermodynamic properties of several hundred hydrocarbons in metric and U. S. Customary units. The data in most instances represent selected values from careful studies, many of which were done in connection with the same API Research Project. Experimental data are supplemented by theoretical calculations or empirical correlations. References to the source data and a bibliography are given.

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- [131] Rossini, F. D., Wagman, D. D., Evans, W. H., Levine, S., and Jaffe, I.  
 Selected Values of Chemical Thermodynamic Properties  
 National Bureau of Standards Circular 500  
 (U. S. Government Printing Office, Washington, D.C., 1952)

This was for many years the most comprehensive authoritative compilation of thermochemical data at 298.15 K for inorganic substances. All inorganic substances and organic substances containing two carbon atoms or fewer per molecule are included if thermodynamic data exist for calculating one of the properties tabulated. Properties tabulated in Part I are  $\Delta_f G^\circ (0)$ ,  $\Delta_f H^\circ (0)$ ,  $\Delta_f H^\circ (298.15 \text{ K})$ ,  $\Delta_f G^\circ (298.15 \text{ K})$ ,  $\log K_f$ ,  $S^\circ (298.15 \text{ K})$ , and  $C^\circ (298.15 \text{ K})$ . Properties tabulated in Part II are temperature, pressure, enthalpy change, entropy change and heat capacity change for transition, fusion, and vaporization processes. The data from original sources were critically evaluated and functions tabulated, maintaining internal consistency by the relationship:  $\Delta_f G^\circ (298.15 \text{ K}) = \Delta_f H^\circ (298.15 \text{ K}) - T \Delta_f S^\circ (298.15 \text{ K})$ . The sources of data for each data item are listed and a bibliography is included. Part I has been superseded by the NBS Tables of Chemical Thermodynamic Properties (see [149]). Much of the data in Part II cannot be found readily elsewhere.

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- [132] Saline Water Conversion Engineering Data Book - 1975  
 (National Technical Information Service, Springfield, Virginia, 1975)

This very large (707 pages) book was produced by the M. W. Kellogg Company for the Office of Saline Water of the U. S. Department of the Interior. The book contains a large amount of miscellaneous engineering information pertinent to examples of engineering and cost calculations, materials of construction, and process flow diagrams for distillation, freezing, reverse osmosis, and electrodialysis. Included in the tables of physical property data are heat capacities, enthalpies, vapor pressures, solubilities, equilibrium constants, critical properties, and mechanical and transport properties. Materials of interest include sea water and aqueous solutions formed from sodium chloride, magnesium chloride, calcium sulfate, calcium carbonate, magnesium sulfate, and hydrocarbons. Much of the data is presented in graphical form with references to the source from which it was taken.

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- [133] Sanderson, R. T.  
 Chemical Bonds and Bond Energy  
 (Academic Press, New York and London, 1971)

This book contains a general discussion of the calculation of bond energies and gives details of calculations performed on 850 different kinds of bonds in more than 500 compounds. Although the bond energies refer to the gaseous state, they are still useful in applications to aqueous systems. The Appendix contains a table of bond energies and enthalpies of formation. The chemical bonds are both inorganic and organic in nature. Also see items [11] and [92].

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- [134] Schmidt, E.  
Properties of Water and Steam in SI Units  
(Springer-Verlag, Berlin, 1982)

This book contains tables of the properties of water and steam from 0 to 800 °C and from 0 to 1000 bar which have been calculated using a set of equations accepted by the members of the Sixth International Conference on the Properties of Steam in 1967. Properties which are tabulated include the pressure, specific volume, density, specific enthalpy, specific heat of evaporation, specific entropy, specific isobaric heat capacity, dynamic viscosity, thermal conductivity, the Prandtl number, the ion-product of water, the dielectric constant, the isentropic exponent, the surface tension and Laplace coefficient. Also see items [43] and [70].

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- [135] Serjeant, E. P. and Dempsey, B.  
Ionization Constants of Organic Acids in Aqueous Solution  
(Pergamon Press, New York, 1979)

This critical compilation of pK values is a supplement to an earlier monograph by Kortum, Vogel, and Andrussov (see item [73]). This volume extends the literature coverage to the end of 1970 and summarizes data for some 4500 acids. In conjunction with the Kortum compilation, the total number of acids covered is  $\approx 5500$ . Each entry includes the name of the substance, its molecular formula, pK value; the temperature, method of measurement, an assessment of reliability, and references to the literature.

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- [136] Silcock, H. (editor) Solubilities of Inorganic and Organic Compounds (in three volumes) (Pergamon Press, Oxford, 1979)  
Translated from the Russian: "Spravochnik po rastvorimosti"  
(Izdatel'stvo Nauka, Moscow, 1969)

This three volume series is an extension of the work of Stephen and Stephen (see item [142]). These volumes cover ternary and multicomponent systems of inorganic substances.

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- [137] Sillen, L. G. and Martell, A. E.  
Stability Constants of Metal Ion Complexes, Section I: Inorganic Ligands,  
Section II: Organic Ligands (Second edition)  
(Special Publication No. 17, The Chemical Society, London, 1964  
and Supplement No. 1, Special Publication No. 25, 1971)

With the publication of this second edition of Stability Constants, the Chemical Society combined two previously separate volumes into one, two-part volume (745 pp.), the first covering constants of inorganic ligands, the second, organic ligands. Both sections include all data published up to the end of 1960 and some from 1961 to 1963; the scope of the inorganic section has been extended to cover redox equilibria and the extraction of inorganic

ligands into nonaqueous solvents. The data are organized into separate tables, each table summarizing the data for the association of one particular ligand with all the metallic ions which have been studied in conjunction with it. Method of measurement, composition, and temperature of the media to which the data refer, are given for each ligand-metal pair. Acid dissociation constants of the ligands are recorded by including the hydrogen ion as one of the cations with which the ligands associate. Redox equilibria are represented by including the electron as a ligand, and hydrolysis of metallic ions is described by regarding the hydroxyl ion as one of the ligands.

The arrangement of material is now more uniform than in the two parts of the first edition, but there remain minor differences of presentation between the inorganic and the organic section. In the inorganic table, 80 ligands are ordered according to group in the periodic system; metal ions are arranged within each inorganic ligand table, in the same order. In the organic section, the ligands (1028) are in order of their empirical formulae, and the metallic ions in the alphabetical order of their international symbols. Methods of measurement are given, with 42 separate methods alphabetized and coded in the introduction; the medium is usually aqueous. Equilibrium constants are given in both tables. The organic section includes consecutive or stepwise constants,  $K$ , whenever possible, and cumulative or gross constants,  $\beta$ , if they are the only quantities determined, or if the sequence of stepwise constants is incomplete. The inorganic table includes equilibrium constants for consecutive and cumulative reactions, solubility constants, acid constants and base constants. Certain special constants are also given; e.g.  $K_D$  - equilibria involving a gas. Both tables give enthalpy and entropy changes, and symbols relating to the references which are listed at the end of each table. Each of the metals, inorganic ligands and organic ligands are indexed alphabetically, with appropriate table number, at the end of the book.

The first edition was authored by J. Bjerrum, G. Schwarzenbach, and L. G. Sillen and was published in two parts by the Chemical Society of London: (1) "Organic Ligands," Special Publication No. 6 (1957) and "Inorganic Ligands," Special Publication No. 7 (1958).

The supplement to the second edition of "Stability Constants of Metal-Ion Complexes" is a review of pertinent literature published between the completion of the 1964 Tables and the end of 1968, including also some data published before the completion of the 1964 Tables, but omitted from them. In the organic part, a change of policy has been initiated; rather than being omitted, results seeming incomplete or of dubious validity are now included in the tables, with critical comments. The section "How to Use the Tables" has been brought up-to-date; a few methods have been added. Limits of error are now sometimes given. A new feature in the organic section is a Functional Group Index, covering also the 1964 Tables, and a table of 34 macromolecular organic ligands, including albumin, DNA, RNA, and insulin. Also see item [89] for the continuation of these compilations by Martell and Smith.

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- [138] Skinner, H. A. (editor)  
MTP International Review of Science - Volume 10  
Thermochemistry and Thermodynamics  
(Butterworths, London, 1972)

Although this book contains few tables of thermodynamic data, it does contain several chapters of interest. These chapters are:

<u>Author(s)</u>	<u>Chapter</u>
I. Wadsö	Biochemical Thermochemistry
R. F. Jameson	Thermodynamics of Metal-Complex Formation
G. Pilcher	Thermochemistry of Chemical Compounds
K. P. Mishchenko	Thermodynamics of Electrolyte Solutions
B. J. Zwolinski and J. Chao	Critically Evaluated Tables of Thermodynamic Data

The last article provides a very useful guide to much of the evaluated thermodynamic data that are not covered in this bibliography.

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- [139] Smith-Magowan, D. and Goldberg, R. N. A Bibliography of Sources of Experimental Data Leading to Thermal Properties of Binary Aqueous Electrolyte Solutions (NBS Special Publication 537, U.S. Government Printing Office, Washington, D.C., 1979)

This is a bibliography of sources of experimental data that can be used to calculate either relative apparent molar enthalpies or apparent molar heat capacities of aqueous electrolyte solutions. The compounds are arranged according to the standard thermochemical order of arrangement. There are approximately 300 references to the source literature.

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- [140] Sober, H. A. (editor)  
Handbook of Biochemistry-Selected Data for Molecular Biology  
(The Chemical Rubber Co., Cleveland, Ohio, 1968)

This compendium contains the following twenty-three tables of thermochemical data. This Handbook appeared in revised form in 1976 (see item [34]):

<u>Author(s) or Source</u>	<u>Table</u>
From "The Chemistry of the Amino Acids and Proteins," C.L.A. Schmidt (editor) Charles C. Thomas Co., Springfield, IL	Coefficients of Solubility Equations of Certain Amino Acids in Water (Section B, page B-3)

Solubility data for 34 amino acids are fitted to equations giving the solubility as a function of temperature.

J. O. Hutchens

Heat Capacities, Absolute Entropies  
and Entropies of Formation of Amino  
Acids and Related Compounds  
(Section B, page B-5)

$C_p^\circ$ ,  $S^\circ$ , and  $\Delta_f S^\circ$  at 25 °C are tabulated for 28 amino acids, 3 peptides,  
4<sup>P</sup>proteins, and 3 related substances.

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J. O. Hutchens and E. P. K. Hade, Jr.

Solubilities of Amino Acids in Water  
at Various Temperatures  
(Section B, page B-10)

The solubilities of 18 amino acids are tabulated at four different temperatures  
from 1 to 40 °C.

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J. O. Hutchens

Heats of Combustion, Enthalpy and  
Free Energy of Formation of Amino  
Acids and Related Compounds  
(Section B, page B-7)

Enthalpies of combustion and formation and Gibbs energies of formation  
at 25 °C are tabulated for 45 amino acids and related compounds.

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J. O. Hutchens

Heats of Solution of Amino Acids in  
Aqueous Solution at 25 °C  
(Section B, page B-11)

The heats of solution for 37 amino acids at 25 °C are tabulated.

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J. O. Hutchens

Free Energies of Solution and Standard  
Free Energies of Formation of Amino  
Acids in Aqueous Solution at 25 °C  
(Section B, page B-13)

Gibbs energies of solution and formation at 25 °C are given for 18 amino acids.

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J. O. Hutchens

Activities of Amino Acids and  
Peptides at 25 °C  
(Section B, page B-14)

Molar activity coefficients at 25 °C are tabulated as a function of molality  
for 14 amino acids.

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From K. S. Markley, "Fatty Acids.  
Part I," second edition,  
Interscience, New York (1960)

Solubility of Fatty Acids in Water  
(Section E, page E-13)

The solubilities of 13 fatty acids in water at five temperatures from 0 to 60 °C are tabulated.

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From K. S. Markley, "Fatty Acids.  
Part I," second edition,  
Interscience, New York (1960)

Approximate Solubilities of Water  
in Saturated Fatty Acids at Various  
Temperatures  
(Section E, page E-13)

The approximate solubilities of water in thirteen saturated fatty acids at various temperatures is given.

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From K. S. Markley, "Fatty Acids.  
Part I," second edition,  
Interscience, New York (1960)

Solubility of Simple Saturated  
Triglycerides  
(Section E, page E-14)

Tabulated are solubilities of five saturated triglycerides in various non-aqueous solvents and at a variety of temperatures.

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From K. S. Markley, "Fatty Acids.  
Part I," second edition,  
Interscience, New York (1960)

Solubilities of Mixed Triacid  
Triglycerides at 25 °C  
(Section E, page E-15)

Solubilities of four mixed triacid triglycerides in four non-aqueous solvents are tabulated.

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P. A. Loach

Oxidation-Reduction Potentials,  
Absorbance Bands and Molar  
Absorbance of Compounds in  
Biochemical Studies  
(Section J, page J-27)

Oxidation-reduction potentials at ambient temperatures are tabulated for an assortment of 253 couples frequently encountered in biochemical studies with appropriate references.

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R. W. Henderson and T. C. Morton

Oxidation-Reduction Potentials of  
Hemoproteins and Metalloporphyrins  
(Section J, page J-35)

Oxidation-reduction potentials are tabulated for 241 hemoproteins and metalloporphyrins at various temperatures.

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R. M. Izatt and J. J. Christensen

Heats of Proton Ionization and  
Related Thermodynamic Quantities  
(Section J, page J-49)

This section is an extensive tabulation of enthalpy and entropy changes and pK values for organic and biochemical systems with 323 references to the literature.

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G. C. Krescheck

Calorimetric  $\Delta H$  Values Accompanying  
Conformational Changes of Macro-  
molecules in Solution  
(Section J, page J-140)

Tabulated are  $\Delta H$  values accompanying the conformation changes of 25 macromolecular systems.

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W. P. Jencks

Free Energies of Hydrolysis and  
Decarboxylation  
(Section J, page J-144)

A discussion is given of standard states appropriate to biochemical thermodynamics. Tabulated are Gibbs energies of hydrolysis of esters of acetic acid and related compounds, of thiol esters, amides, phosphates, and of glycolysis (and of decarboxylation).

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W. P. Jencks and J. Regenstein

Ionization Constants of Acids  
and Bases  
(Section J, page J-151)

Given is an extensive tabulation of pK values for ionization of several hundred acids and bases with 116 references to the literature.

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R. G. Bates

Measurement of pH  
(Section J, page J-190)  
and  
Buffer Solutions  
(Section J, page J-195)

pH values have been assigned to several important buffer systems.

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N. F. Good, G. D. Winget, W. Winter,  
T. N. Connolly, S. Izawa, and R. M. M. Singh,  
5, 472 (1966)

Properties of Some New  
Buffers for Biochemistry  
Biological Research  
(Section J, page J-195)

Tabulated are pK values with temperature coefficients and metal-buffer binding constants for several buffers useful for biological research.

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- [141] Stary, J. and Freiser, H.  
Equilibrium Constants of Liquid-Liquid Distribution Reactions.  
Part IV: Chelating Extractants  
(Pergamon Press, Oxford and New York, 1978)

This 228 page volume summarizes equilibrium constants for liquid-liquid distribution equilibrium constants up to the end of 1972. Each table includes: the extractant and its extractable metal complexes, and the distribution equilibrium constants and extraction constants. The aqueous phase metal complex formation constants are not included and the reader is referred to items and in this bibliography for sources of this type of data. References to the primary literature are included.

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- [142] Stephen, H. and Stephen, T. (editors)  
Solubilities of Inorganic and Organic Compounds (in five volumes)  
(Pergamon Press, Oxford, 1963 and 1964)

This series, which has been translated from the Russian, consists of five volumes (about 5500 pages) and is a selection from the literature of data on the solubilities of elements, inorganic compounds, and organic compounds in binary, ternary, and multi-component systems. References are given to sources of data in the literature. The data are unevaluated and refer to temperatures for which experimental data exist. Also see the three volume extension edited by Silcock [136].

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- [143] Stull, D. R.  
Vapor Pressure of Pure Substances. Organic Compounds  
Industrial and Engineering Chemistry 39, 517 (1947)  
and  
Vapor Pressure of Pure Substances. Inorganic Compounds  
Industrial and Engineering Chemistry 39, 540 (1947)

These articles contain evaluated vapor pressure data on over 1200 organic and 300 inorganic compounds. Given for each compound are those temperatures at which the compounds has a given vapor pressure.

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- [144] Stull, D.R. and Prophet, H. (project directors) JANAF Thermochemical Tables (second edition) NSRDS-NBS 37 (U.S. Government Printing Office, Washington, D.C., 1971)

This extensive volume contains values of  $C_p^\circ$ ,  $S^\circ$ ,  $(G^\circ - H^\circ(298.15\text{ K}))/T$ ,  $H^\circ - H^\circ(298.15\text{ K})$ ,  $\Delta_f H^\circ$ ,  $\Delta_f G^\circ$ , and  $\log_{10} K$ , where  $K$  is the equilibrium constant for the reaction of forming the given compound from its elements. The temperature range for which the data are given is 0 K to the highest temperature for which the data exist, the temperature intervals being in steps of 100 K. For each compound given there is a concise and detailed discussion of the data upon which the accompanying table is based and references to the source literature. The volume contains data for  $\approx 1200$  elements and compounds in the crystalline, liquid and gaseous states. It should be noted that the reference state for phosphorus is the red form. While most of the substances are inorganic, there is also some coverage of organic materials up to five carbon atoms. Three supplements to the JANAF tables have appeared in the Journal of Physical and Chemical Reference Data for a total of 1322 tabulations involving 35 elements and their compounds. Also see [42]. The supplements are:

<u>Author(s)</u>	<u>Reference</u>
M.W. Chase, Jr., J.L. Curnutt, A.T. Hu H. Prophet, A.N. Syverud and L.C. Walker	Journal of Physical and Chemical Reference Data <u>3</u> , 311 (1974).
M.W. Chase, Jr., J.L. Curnutt, H. Prophet R.A. McDonald and A.N. Syverud	Ibid <u>4</u> , 1 (1975)
M.W. Chase, Jr., J.L. Curnutt, R.A. McDonald and A.N. Syverud	Ibid <u>7</u> , 793 (1978)
M.W. Chase, Jr., J.L. Curnutt, J.R. Downey, Jr., R.A. McDonald, A.N. Syverud, and E.A. Valenzuela	Ibid <u>11</u> , 695 (1982)

\* \* \* \* \*

- [145] Stull, D. R., Westrum, E. F. and Sinke, G. C.  
The Chemical Thermodynamics of Organic Compounds  
(John Wiley and Sons, New York, 1969)

This monograph is divided into three parts. The first part gives the theoretical basis and principles of thermodynamics and thermochemistry, some experimental and computational methods used, and some applications to industrial problems. The second part gives thermal and thermochemical properties in the ideal gas state from 298.15 to 1000 K. In this section, the sources of data are listed and discussed and standardized tables are presented for 918 organic compounds. Values of  $C_p^\circ$ ,  $S^\circ$ ,  $-(G^\circ - H^\circ(298.15\text{ K}))/T$ ,  $H^\circ - H^\circ(298.15\text{ K})$ ,  $\Delta_f H^\circ$ ,  $\Delta_f G^\circ$ , and  $\log K_p$  are given enthalpy of formation, entropy, and consistent values of  $\Delta_f G^\circ$  and  $\log K_p$  of organic compounds at 298.15 K. In excess of 4000 compounds are listed, including a few inorganic compounds. In one chapter there is a brief discussion of methods of estimating thermodynamic quantities.

\* \* \* \* \*



- [146] Tatevskii, V. M., Benderskii, V. A. and Yarovoi, S. S.  
 Rules and Methods for Calculating the Physico-Chemical Properties of  
 Paraffinic Hydrocarbons  
 (Pergamon Press, New York and Oxford, 1961)  
 Translated from the Russian:  
 "Zakonomernosti i metody rascheta fizikokhimicheskikh svoisty  
 parafionvykh uglevodorodov"  
 (Gostoptekhizdat, Moscow, 1960)

This monograph is a summary and a consolidation of the results of some years of work by Tatevskii and others, extending and elaborating some procedures introduced by Rossini and others. Properties calculated include: molar volume, molar refraction, vapor pressure, enthalpy of formation from atoms or elements, Gibbs energy of formation, and enthalpy of combustion. Three different methods are used. Tables of constants and illustrations of the accuracy of the methods are given.

\* \* \* \* \*

- [147] Timmermans, J.  
 Physico-Chemical Constants of Pure Organic Compounds (in two volumes)  
 (Elsevier, Amsterdam, 1950 and 1965)

These two volumes contain tables of physical data for pure organic compounds. The arrangement of the data is by compound. Properties tabulated include vapor pressure, boiling point, triple point, viscosity, specific heat, critical constants, density, compressibility, refractive index, enthalpy of vaporization, and dielectric constant.

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- [148] Timmermans, J.  
 The Physico-Chemical Constants of Binary Systems in Concentrated Solutions  
 (in four volumes)  
 (John Wiley and Sons, Interscience Publishers, New York, 1959)

These volumes contain extensive tabulations of physical data relevant to concentrated solutions of binary systems, both organic and inorganic. The properties that are tabulated include dielectric constant, viscosity, equivalent conductivity, surface tension, diffusion and thermal diffusion coefficients, vapor pressure, specific heat, electrochemical data, enthalpy of combustion, enthalpy of dilution and solution, transition enthalpies, and other properties. These books contain extensive tabulations of data pertinent to water and electrolyte solutions. The data are well organized and there is a general compound index as well as references to the original data sources. The literature coverage is through the year 1957.

\* \* \* \* \*

- [149] Wagman, D. D., Evans, W. H., Parker, V. B., Schumm, R. H.,  
 Halow, I., Bailey, S. M., Churney, K. L., and Nuttall, R. L.  
 The NBS Tables of Chemical Thermodynamic Properties  
 Journal of Physical and Chemical Reference Data 11, Supplement No. 2  
 (1982)

This 392 page volume is the most recent comprehensive compilation in English of critically evaluated thermochemical data at 298.15 K for inorganic substances and for organic substances containing one or two carbon atoms. The values are in joules and refer to a standard state of 0.1 MPa. The coverage is approximately 14,000 substances. The properties tabulated are  $\Delta_f H^\circ (0)$ ,  $\Delta_f G^\circ (298.15 \text{ K})$ ,  $\Delta_f H^\circ (298.15 \text{ K})$ ,  $H^\circ (298.15 \text{ K}) - H^\circ (0)$ ,  $S^\circ (298.15 \text{ K})$ , and  $C_p^\circ (298.15 \text{ K})$ . The data from original sources have been critically evaluated and "best" values selected for the properties tabulated, maintaining internal consistency by the relationships  $\Delta_f G^\circ (298.15 \text{ K}) = \Delta_f H^\circ (298.15 \text{ K}) - T\Delta_f S^\circ (298.15 \text{ K})$ , and  $\Delta_f H^\circ (298.15 \text{ K}) - \Delta_f H^\circ (0) = \sum (H^\circ (298.15 \text{ K}) - H^\circ (0))_f$ . This volume contains an excellent discussion dealing with the construction, use, and history of thermochemical tables. This volume supersedes NBS Circular 500 (item [131]). Also see item [93].

The NBS Tables of Chemical Thermodynamic Properties is a new edition of NBS Technical Note 270, "Selected Values of Chemical Thermodynamic Properties." The values in the Technical Notes were in calories and refer to a standard state of one atmosphere. The 1982 NBS Tables also contain some changes, additions, and corrections to the Technical Note. Although superseded by the 1982 NBS Tables, the NBS Technical Note 270 is still relevant to thermochemists since many papers in the literature from the years 1965 to 1982 made use of the values tabulated in the Technical Note. The Technical Note was issued in eight parts from 1965 to 1981 and was published by the U.S. Government Printing Office, Washington, D.C. The parts of the Technical Note, the years of publication and their contents are:

<u>Technical Note</u>	<u>Authors</u>	<u>Year of Publication</u>
270-1	Wagman, D. D., Evans, W. H., Parker, V. B., Halow, I., Bailey, S. M., and Schumm, R. H.	1965

Tables for the elements O, H, He, Ne, Ar, Kr, Xe, Rn, F, Cl, Br, I, At, S, Se, Te, Po, N, P, As, Sb, Bi, and C.

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270-2	Wagman, D. D., Evans, W. H., Halow, I., Parker, V. B., Bailey, S. M., and Schumm, R. H.	1966
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Tables for the elements Si, Ge, Sn, Pb, B, Al, Ga, In, and Tl.

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270-3	Wagman, D. D., Evans, W. H., Parker, V. B., Halow, I., Bailey, S. M., and Schumm, R. H.	1968
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This part combined parts 1 and 2 into one volume and superseded them. Tables for Zn and Cd were also added.

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270-4                    Wagman, D. D., Evans, W. H., Parker, V. B.                    1969  
                          Halow, I., Bailey, S. M., and Schumm, R. H.

Tables for the elements Hg, Cu, Ag, Au, Ni, Co, Fe, Pd, Rh, Ru, Pt, Ir, Os, Mn, Te, Re, Cr, Mo, and W.

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270-5                    Wagman, D. D., Evans, W. H., Parker, V. B.                    1971  
                          Halow, I., Bailey, S. M., Schumm, R. H., and  
                          Churney, K. L.

Tables for the elements V, Nb, Ta, Ti, Zr, Hf, Sc, and Y.

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270-6                    Parker, V. B., Wagman, D. D., and Evans, W. H.                    1971

Tables for the elements Be, Mg, Ca, Sr, Ba, and Ra.

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270-7                    Schumm, R. H., Wagman, D. D., Bailey, S. M.,                    1973  
                          Evans, W. H., and Parker, V. B.

Tables for the elements Lu, Yb, Tm, Er, Ho, Dy, Tb, Gd, Eu, Sm, Pm, Nd, Pr, Ce, and La.

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270-8                    Wagman, D. D., Evans, W. H., Parker, V. B.,                    1981  
                          Schumm, R. H., and Nuttall, R. L.

Tables for the elements U, Pa, Th, Ac, Li, Na, K, Rb, Cs, and Fr. Additions and corrections to the series are given in an appendix.

\* \* \* \* \*

[150] Wagman, D. D., Schumm, R. H. and Parker, V. B.  
       A Computer-Assisted Evaluation of the Thermochemical Data of the  
       Compounds of Thorium  
       (NBSIR 77-1300, National Bureau of Standards, Washington, D.C., 1977)

This report presents a computer-assisted evaluation of the thermochemical properties of compounds of thorium. Values of  $\Delta_f H^\circ$ ,  $\Delta_f G^\circ$ ,  $S^\circ$  are tabulated at 298.15 K for the compounds and aqueous species of thorium. There is also a "reaction catalog" which gives values of  $\Delta G^\circ$ ,  $\Delta H^\circ$ , and  $S^\circ$  for individual processes or substances and upon which the tabulated formation properties are based. This report also contains thermal functions and includes references to the primary literature.

\* \* \* \* \*

- [151] Washburn, E. W. (editor-in-chief)  
International Critical Tables of Numerical Data, Physics, Chemistry,  
and Technology  
(McGraw-Hill Book Company, New York, 1930)

At the time of publication this seven volume series was the most comprehensive source of thermochemical and other data in existence. Essentially all equilibrium and transport properties and classes of materials were covered. The Critical Tables, although now superseded by modern compilations and evaluations of data, still remain useful for references to the older literature. The tables are arranged according to property with groups of tables being arranged according to discipline. One volume of this series is an index of the materials whose properties are dealt with.

\* \* \* \* \*

- [152] Wichterle, I., Linek, J. and Hala, E.  
Vapor-Liquid Equilibrium Data Bibliography (and two Supplements)  
(Elsevier, Amsterdam, 1973, 1976, and 1979)

These three books contain references to the source literature on vapor-liquid equilibrium data for inorganic and organic mixtures. The first volume covers the literature through 1972, the second through 1975, and the third through 1978. The compounds are arranged alphabetically except for the carbon containing compounds. The preparation of the two Supplements has been computerized to make updating more efficient. The series contains 6700 references to the source literature.

\* \* \* \* \*

- [153] Wilhelm, E. Battino, R. and Wilcock, R. J.  
Chemical Reviews 77, 219 (1977)

This paper is a critical review of the low-pressure solubility of 57 gases in liquid water and in heavy water. The solubility of each gas is given in terms of the coefficients of an equation which can be used to calculate the solubility at a given temperature. Also given are  $\Delta G^\circ$ ,  $\Delta H^\circ$ ,  $\Delta S^\circ$ , and  $\Delta C_p^\circ$  values for the solution process at various temperatures and at one atmosphere partial pressure of the gas. The authors give extensive details concerning their correlations and include references to the literature.

\* \* \* \* \*

- [154] Wilhelm, E. and Battino, R.  
Thermodynamic Functions of the Solubilities of Gases in Liquids at 25 °C  
Chemical Reviews 73, 1 (1973)

This review article contains selected values for the solubility, entropy, and enthalpy changes in solution for 16 gases in 39 non-aqueous solvents. Also given are the coefficients of polynomial expressions for the Gibbs energy of solution for a gas in a given solvent as a function of temperature. See also item [8].

\* \* \* \* \*



- [155] Wilhoit, R. C. and Zwolinski, B. J.  
Handbook on Vapor Pressures and Heats of Vaporization of Hydrocarbons  
and Related Compounds (API 44 - TRC)  
(Thermodynamics Research Center, Texas A and M Research Foundation,  
College Station, Texas, 1971)

This handbook gives data for 680 hydrocarbons, 95 carbon-sulfur compounds, and water from 0 to 150 °C. It is indexed by compound name, and by boiling point.

\* \* \* \* \*

- [156] Wilhoit, R. C. and Zwolinski, B. J.  
Physical and Thermodynamic Properties of Aliphatic Alcohols  
Journal of Physical and Chemical Reference Data, Volume 2,  
Supplement No. 1, 1973

This review contains critically evaluated values of the vapor pressure, heat capacity, enthalpies of transition, entropies, thermodynamic functions for the real and ideal gases, densities, refractive indexes, and critical properties for 722 alcohols in the carbon range  $C_1$  to  $C_{50}$ . This comprehensive review is 420 pages long and lists 2036 references.

\* \* \* \* \*

- [157] Wisniak, J.  
Phase Diagrams, A Literature Source Book (Parts A and B)  
(Elsevier, New York, 1981)

These two volumes contain extensive references (circa 18,000) to phase diagrams in the literature. The systems covered include organic and inorganic materials and aqueous systems. The coverage extends over the entire periodic chart. The systems are arranged in order of increasing carbon and hydrogen with the remaining elements in alphabetical order.

\* \* \* \* \*

- [158] Wisniak, J. and Tamir, A.  
Mixing and Excess Thermodynamic Properties: A Literature Source Book  
(Elsevier, Amsterdam, 1978)

This book contains approximately 6000 references to excess mixing property data for mixtures of all types, including electrolyte, non-electrolyte, and metallurgical systems. The appropriate references to the literature are given for each mixture. The coverage of materials encompasses the entire periodic chart and also includes ternary, quaternary, and multi-component mixtures.

\* \* \* \* \*

- [159] Wu, Y. C. and Hamer, W. J.  
Electrochemical Data. Part XIV. Osmotic Coefficients and Mean Activity Coefficient of a Series of Uni-Bivalent and Bi-Univalent Electrolytes in Aqueous Solutions at 25 °C. Part XVI. Osmotic Coefficients and Mean Activity Coefficients of a Number of Uni-Trivalent and Tri-Univalent Electrolytes in Aqueous Solution at 25 °C  
(NBSIR No. 10052 and 10088, National Bureau of Standards, 1969)

These reports give values for the osmotic and mean ionic activity coefficients of uni-bivalent, bi-valent, uni-trivalent, and tri-univalent electrolytes in aqueous solution at 25 °C. In each case, the values tabulated are those calculated by fitting the literature data to the equation for the excess Gibbs energy, and represents a good fit to the experimental data. Literature references are included. Also see item [48].

\* \* \* \* \*

- [160] Yatsimirskii (or Jazimirski), K. B.  
 Thermochemie von Komplexverbindungen  
 (Akademie-Verlag, Berlin, 1956)  
 translated by Georg Crull from the Russian  
 "Thermochimia Complexnik Coedinenie"  
 (Akad. Nauk. CCCP, Moscow, 1951)

This monograph contains correlations of thermochemical data of complex compounds in terms of gas, crystal, and solution models emphasizing ionic radii. More than 1400 substances are considered. In summary tables, 52 metal cations, 33 neutral ligands, and 25 anions have enthalpies of formation listed, usually for gaseous and aqueous state. The compounds formed from these ions and ligands are listed usually with the enthalpy of formation of the crystal, and for many of them enthalpies of solution at infinite dilution are given. The chapters discuss and give tables and correlations of hydration enthalpies of cations, anions and some amine salts, ion entropies in solution, enthalpies of formation and solution, energies of gas and crystal ions, binding energies of  $H_2O$ ,  $NH_3$  and other molecules to central metal ions in gaseous complex ions and similar binding energies.

\* \* \* \* \*

- [161] Yatsimirskii, K. B., and Vasil'ev, V. P.  
 Instability Constants of Complex Compounds  
 (Consultants Bureau, New York, 1966 and Pergamon Press, New York, 1960)

This volume contains an extensive tabulation of equilibrium data ( $K$  and  $-\log K$ ) and enthalpies of formation for processes involving the more common ions and ligands in aqueous solution. Specified are the temperature, ionic strength, and method of measurement with reference(s) to the appropriate literature. The tables contain instability constants for 138 predominantly inorganic complexes.

\* \* \* \* \*

- [162] Kerr, J. A.  
 Strengths of Chemical Bonds  
 in CRC Handbook of Chemistry and Physics, 64th Edition, 1983-1984  
 (CRC Press, Inc., Boca Raton, Florida, 1983)

This 20 page compilation (pages F-176 to F-195 in the "Handbook of Chemistry and Physics") contains values of bond strength in diatomic and polyatomic molecules, enthalpies of formation of gaseous atoms from the elements in their standard states, and enthalpies of formation of free radicals. The data refer to 298.15 K. The coverage of bond types is extensive and there are references to the source literature. Also see item [92].

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## SUBJECT INDEX

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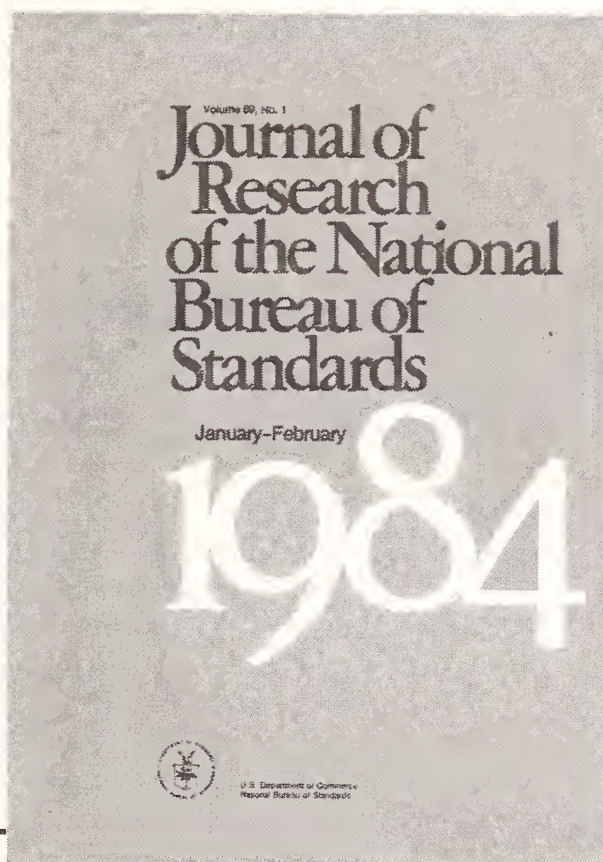
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