An Annotated Bibliography of Compiled Thermodynamic Data Sources for Biochemical and Aqueous Systems (1930 to 1975)

Equilibrium, Enthalpy, Heat Capacity, and Entropy Data

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Office of Standard Reference Data — Office of Information Activities — Office of Technical Publications — Library — Office of International Relations — Office of International Standards.

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[1] Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.

[2] Located at Boulder, Colorado 80302.

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Equilibrium, Enthalpy, Heat Capacity, and Entropy Data

special publication, no. 4

George T. Armstrong and Robert N. Goldberg

Institute for Materials Research
National Bureau of Standards
Washington, D.C. 20234

National Bureau of Standards Special Publication 454

Foreword

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

The task of critical evaluation is carried out in various data centers, each with a well-defined technical scope. A necessary preliminary step to the critical evaluation process is the retrieval from the world scientific literature of all papers falling within the scope of the center. Each center, therefore, builds up a comprehensive well-indexed bibliographical file which forms the base for the evaluation task. Bibliographies derived from these files are published when they appear to be of value to research workers and others interested in the particular technical or programmatic area.

The present effort provides a useful collection of data sources required in solving problems associated with water pollution. The properties data extracted from the bibliographic sources cited in this document will help classify the behavior of many of the specific pollutants found in the water environment.

Further information on NSRDS and the publications which form the primary output of the program may be obtained by writing to the Office of Standard Reference Data, National Bureau of Standards, Washington, D.C. 20234

David R. Lide, Jr., Chief
Office of Standard Reference Data

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"The cold tables of physical and chemical constants, the base equations in textbooks, form the hardcore, the residue distilled from individual triumphs of insight, checked and cross-checked by the multiple testimony of general experience"

Gerald Holton
American Scientist, 41, 93 (1953)

ABSTRACT

Contained herein 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 molal 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; Gibbs energy data; heat capacity data; partial molal properties; thermochemistry; thermodynamics; review articles; water pollution.

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 decidely 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 NSRDS, CODATA, and other coordinating organizations are providing current compilations. However, the preparation of new reviews is sufficiently complex that there are at any given 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 entries of the bibliography are listed in alphabetical order by leading author. A brief description of the contents of each is given to permit the reader to select those references which will most directly apply to his own needs. Some of the compilations (I) were prepared specifically for use in biochemical or aqueous solution thermodynamics, while others (were prepared for a more general thermodynamic audience, but also contain substantial amounts of data valuable to these two areas; others (III) are of tangential interest and contain some, but comparatively limited amounts of data specific to either biochemical or aqueous systems. These three degrees of relevance are indicated by the Roman numerals I, II, and III, respectively. Thus, each entry in this bibliography will have associated with it two Roman numerals, the first referring to its relevancy with regards to biochemical systems and the latter with regard to aqueous systems. This bibliography is intended to be fairly complete with respect to categories I and II but makes no attempt at completeness in category III. The authors would appreciate comments from interested readers concerning data sources omitted from this bibliography.

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.

1. Alberty, R. A.   I, II
    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. A critical evaluation of the relevant literature data is included.

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2. Armstrong, G. T., Domalski, E. S., Furukawa, G. T., Reilly, M. L.,   I, II
    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, DC   20234)

This series of reports is a survey of the thermodynamic properties of selected compounds of
biological importance containing the elements carbon, hydrogen, nitrogen, oxygen,
phosphorous, 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. References to sources of data in the literature are included.

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3. Ashcroft, S. J., and Mortimer, C. T.   II, I
    Thermochemistry of Transition Metal Complexes
    (Academic Press, London, 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 ΔH, ΔG, and ΔS for various stages
of complex formation are usually listed for processes in aqueous solution. $\Delta E_f°$, $\Delta G_f°$, $\Delta S_f°$
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.

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Baes, C. F., Jr., and Mesmer, R. E. -- see entry no. 93
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Bates, R. G. -- see entry no. 94
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4. Battino, R.   III, I
    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 molal 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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5. Battino, R., and Clever, H. L.   III, I
    The Solubility of Gases in Liquids
    Chemical Reviews, <u>66</u>, 395 (1966)

This thorough and detailed review contains a detailed 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.

More recently, E. Wilhelm and R. Battino (Chemical Reviews, <u>73</u>, 1 (1973)) have critically
evaluated the solubilities and enthalpies of solution of gases in non-aqueous solvent
systems.

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6. Benson, S. W.   III, III
    Thermochemical Kinetics
    Methods for the Estimation of Thermochemical Data and Rate Parameters
    (John Wiley and Sons, Inc., New York, London, Sydney, 1968)

This monograph gives tables of necessary data and descriptions of methods of their use for
calculating ΔH_f, Cp, and S at 25 °C for gas phase molecules and radicals and for extra-
polating them to higher temperatures. The procedures can be applied to hydrocarbons,
oxygen-containing compounds, nitrogen-containing compounds, haloalkanes, organo-sulfur
compounds, and organo-metallic compounds, and deal principally with organic compounds.

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7. Benson, S. W., Cruickshank, F. R., Golden, D. M., Haugen, G. R.,   III, III
    O'Neal, H. E., Rogers, A. S., Shaw, R., and Walsh, R.
    Additivity Rules for the Estimation of Thermochemical Properties
    Chemical Reviews, <u>69</u>, 279-324 (1969)

This lengthy technical article gives procedures for calculating the properties $\Delta H_f°$, $S°$,
Cp°, for organic compounds in the gas phase. Parameters for calculating Cp are given for the
temperature range from 300 to 1500 K. The availability of Cp as a function of temperature allow
calculation of $\Delta H_f°$ and $S°$ 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^{-1} (4 kJ·mol^{-1}) or better in $\Delta H_f°$ and
1 cal·mol^{-1}·K^{-1} (4 J·mol^{-1}·K^{-1}) or better in Cp° and $S°$ are generally found.

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8. Bichowsky, F. R., and Rossini, F. D.   II, II
    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 $\Delta H_f°$ 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.
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   Physical Properties of Molecular Crystals, Liquids, and Glasses
   (John Wiley and Sons, Inc., New York, London, Sydney, 1968)

This monograph is designed for the use of chemical engineers to estimate physical properties needed in design calculations, as well as of 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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Boublik, T., Fried, V., and Hala, E. - see entry no. 95

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10. Brown, H. D. (editor)   I, II
    Biochemical Microcalorimetry
    (Academic Press, New York, London, 1969)

This book contains seventeen articles on subjects concerning heat measurements and their relationship to biology and biochemistry. Several of the articles contain tabulations of data:

Author(s)	Title of Article
R. C. Wilhoit	Thermodynamic Properties of Biochemical Substances

This review includes several tables: (1) Selected values of thermodynamic properties (ΔH_f°, ΔG_f°, S°, and Cp°) 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) ΔH° and ΔG° for six important biochemical processes; and (4) Partial molal properties ($\overline{L}_2$, $\overline{L}_1$, $\overline{C}_2$, and $\overline{C}_1$) 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 article has a table of enthalpies of isomerization of eleven carbohydrates and a table giving enthalpies of hydrolysis of aqueous α-1,4 and α-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 |

There is a tabulation of calorimetrically determined enthalpy values accompanying conformational changes of macromolecules in solution (26 references).

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| H. D. Brown | Calorimetry of Enzyme-Catalyzed Reactions |

Tabulated are calorimetric enthalpy values for enzyme catalyzed systems (21 references).

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11. Chapman, T. W., and Newman, J.   III, I

     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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12. Charlot, G.   III, I
     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. Entries are given for about 350 inorganic systems. The literature coverage is
through 1967.

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13. Christensen, J. J., and Izatt, R. M.   II, I
     Handbook of Metal Ligand Heats and Related Thermodynamic Quantities (second edition)
     (Marcel Dekker, Inc., 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 $\log K$, ΔS, and ΔCp, 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
temperature, the method, and conditions of measurement of ΔH are given. 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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14. Christensen, J. J., Eatough, D. J., and Izatt, R. M.   I, II
     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 $\log K$, ΔH, ΔS, and ΔCp data for the
interaction of inorganic cations with synthetic multidentate macrocyclic compounds. Each
entry in the table of thermodynamic data includes the temperature, ionic strength, solvent
system, and method of measurement used in obtaining the data.

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15. Clark, W. M.   I, II
     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 re-
duction potentials for organic and biochemical systems thru 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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16. CODATA Recommended Key Values for Thermodynamics 1975   III, II
     (CODATA Bulletin No. 17 (1976) and Tentative Set of Key Values for Thermodynamics:
     Part V, CODATA Special Report 3, September 1975)

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 $\Delta H_f°$ (298.15 K), $S°$ (298.15 K),
and $H°$ (298.15 K) - $H°$ (0 K) for 102 of the thermochemically more important elements and
compounds, including some aqueous species. These bulletins supersede earlier CODATA reports
of this group. It should be noted that the recommended values are not fully consistent
with any previously published thermodynamic tables, but are intended to form the basis of
future generations of compilations (also see annotation on compilation by Parker, Wagman,
and Garvin).

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17. Coetzee, J. F., and Ritchie, C. D. (editors)   II, I
     Solute-Solvent Interactions
     (Marcel-Dekker, New York and London, 1969).

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

(1) Larson, J. W., and Hepler, L. G., "Heats and Entropies of Ionization". This chapter
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.

(2) Arnett, E. M., and McKelvey, D. R., "Solvent Isotope Effect on Thermodynamics of Non-
reacting Solutes". 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.

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

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18. Conway, B. E.   II, I
     Electrochemical Data
     (Elsevier Publishing Company, 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 molal 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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19. Covington, A. K.   III, I
     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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20. Cox, J. D., and Pilcher, G.   II, III
     Thermochemistry of Organic and Organometallic Compounds
     (Academic Press, London, New York, 1970)

This monograph is a critical compilation of thermochemical data for the title field
published since 1930. The enthalpies of formation 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.

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21. Domalski, E. S.   II, III
     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 $\underline{1}$, 221-277 (1972)

Selected values of the enthalpies of combustion and enthalpies of formation of 719 organic
compounds 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.

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22. Dorsey, N. E.   II, I
     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.

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23. Dymond, J. H., and Smith, E. B.   III, III
     The Virial Coefficients of Gases
     (Clarendon Press, Oxford, 1969)

This book is a critical compilation of the virial coefficients of about 280 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.

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24. Florkin, M., and Mason, H.   I, II
     Comparative Biochemistry, Volume II. Free Energy and Biological Function
     (Academic Press, New York, 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:

M. R. Atkinson and R. K. Morton, "Free Energy and Biosynthesis of Phosphates". 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". 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". 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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25. Fox, D., Labes, M. M., and Weissberger, A. (editors)   II, III
    Physics and Chemistry of the Organic Solid State
    (Interscience Publishers (Wiley), 1963)

E. F. Westrum 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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26. Franks, F. (editor)   II, I
    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:

Authors   Chapter

F. Franks   The Properties of Ice

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
                                       Mixtures

Included is the density of water as a function of temperature, the vapor pressure, specific
heat, partial molal volume, critical properties, and viscosity of water.

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K. Tödheide   Water at High Temperatures and Pressures

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.

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F. Franks and D. S. Reid   Thermodynamic Properties

Given are $\Delta G°$, $\Delta H°$, $\Delta S°$, and $\Delta Cp°$ for the solution of hydrocarbons, alcohols, and rare gases
in water.

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H. L. Friedman and C. V. Krishnan   Thermodynamics of Ionic Hydration

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
molal volumes of about 120 common ions at 25 °C; ionic partial molal heat capacities of ions;
Gibbs energies of transfer of inorganic electrolytes from H_2O to D_2O; and calorimetrically
determined enthalpies of solution of salts in H_2O and D_2O.

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26. (continued)

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

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

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Gedansky, L. M., and Hepler, L. G. -- , see entry no. 96

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27. Glushko, V. P. (editor), Medvedev, V. A., Bergman, G. A., Gurvich, L. V.,   II, II
    and others
    Thermal Constants of Substances (Volumes 1 to 7)
    (In Russian)
    (VINITI, Moscow, 1965 to 1974)

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 $\Delta H_f°$, $\Delta G_f°$, $S°$, 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. In the volumes listed, the elements, in the standard order of arrangement, through hafnium are covered. Carbon and its compounds are covered up to two carbons atom. The coverage and arrangements of substances is similar to that used in the NBS Technical Note 270 series (see Wagman, et al.)

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28. Goldberg, R. N., and Hepler, L. G.   III, II
    Thermochemistry and Oxidation Potentials of the Platinum Group Metals and Their
    Compounds
    Chemical Reviews, 68, 229 (1968)

This article is a critical review and selection of thermochemical data for the platinum group metals and their compounds. Tabulated are selected values of $\Delta H_f°$, $\Delta G_f°$, $S°$, and electrode potentials at 25 °C. There are 212 references to the primary literature.

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29. Hamer, W. J. (editor)   III, I
    The Structure of Electrolytic Solutions
    (John Wiley and Sons, Inc., New York, 1959)

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

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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29. (continued)

<u>Authors</u>   <u>Chapter</u>

E. Lange   Heats of Dilution of Dilute Solutions of
                                            Strong and Weak Electrolytes

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.**

H. S. Harned   Diffusion and Activity Coefficients of
                                            Electrolytes in Dilute Aqueous Solutions

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

F. H. Spedding and G. Atkinson   Properties of Rare Earth Salts in Electrolytic
                                            Solutions

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

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30. Hamer, W. J., and DeWane, H. J.   III, I
    Electrolytic Conductance and the Conductances of the Halogen Acids in Water
    (NSRDS-NBS 33, U. S. Government Printing Office, Washington, DC, 1970)

This monograph contains a detailed evaluation of equivalent conductance data for hydrofluoric,
hydrochloric, hydrobromic, and hydroiodic acids in water over wide ranges of temperature and
concentration.

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31. Hamer, W. J., and Wu, Y. C.   III, I
    The Activity Coefficients of Hydrofluoric Acid in Water from 0 to 35 °C
    Journal of Research of the National Bureau of Standards, <u>74A</u>, 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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32. Hamer, W. J., and Wu, Y. C.   III, I
    Osmotic Coefficients and Mean Activity Coefficients of Uni-univalent Electrolytes in
    Water at 25 °C
    Journal of Chemical Reference Data, <u>1</u>, 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

32. (continued)

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 concentra-
tion. Literature references are given to fifty-one additional uni-univalent electrolytes.

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33. Harned, H. S., and Owen, B. B.   III, I
     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 molal heat contents, activity coefficients,
pH values, densities, and activity coefficients for many of the more common inorganic and
organic electrolyte solutions.

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34. Harned, H. S., and Robinson, R. A.   III, I
     Multicomponent Electrolyte Solutions
     (Pergammon 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 inter-
pretation 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 and which deal with electrolyte solution:

Author	Title 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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35. Hawkins, D. T.   III, I
     A Bibliography on the Physical and Chemical Properties of Water
     Journal of Solution Chemistry, $\underline{4}$, 621 (1975)

This bibliography consists of 1999 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 1969 to 1974. An earlier bibliography covering the years 1957 to 1968 was also issued,
but is now out-of-print. These two bibliographies have recently been combined and should be
available from Plenum Press in 1976.

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36. Hepler, L. G., and Olofsson, G.   III, II
    Mercury: Thermodynamic Properties, Chemical Equilibria, and Standard Potentials
    Chemical Reviews, $\underline{75}$, 585 (1975)

This article is a critical review and selection of thermochemical data for mercury and
about 130 of its compounds primarily inorganic but including many aqueous species.
Tabulated are selected values of $\Delta G_f°$, $\Delta H_f°$, $S°$, electrode potentials, and selected
equilibrium constants at 25 °C. There are 251 references to the primary literature.

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37. Hill, J. O., Worsley, I. G., and Hepler, L. G.   III, II
    Thermochemistry and Oxidation Potentials of Vanadium, Niobium, and Tantalum
    Chemical Reviews, $\underline{71}$, 127 (1971)

This article is a critical review and contains a careful selection of thermochemical data
for vanadium, niobium, and tantalum and about 110 of their compounds, including some aqueous
species. Tabulated are selected values of $\Delta G_f°$, $\Delta H_f°$, $S°$, and electrode potentials at
25 °C. There are 121 references to the primary literature.

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Ingraham, L. L., and Pardee, A. B. -- see entry no. 97

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38. Izatt, R. M., Christensen, J. J., and Rytting, J. H.   I, II
    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, $\underline{71}$, 439 (1971)

This review contains twenty-three journal pages of tables of thermodynamic data ($\log K$, ΔH,
ΔS, and ΔCp) 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 to
articles in the literature.

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39. Janz, G. J.   III, III
    Thermodynamic Properties of Organic Compounds
    Estimation Methods, Principles, and Practice (revised edition)
    (Academic Press, Inc., New York, 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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40. Janz, G. J., and Tomkins, R. P. T.   III, III
    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° 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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Jazimirski (Yatsimiraskii), K. B. -- see entry no. 98
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41. Jordan, T. E.   III, III
    Vapor Pressure of Organic Compounds
    (Interscience Publishers, Inc., 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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42. Joshi, R. M., and Zwolinski, B. J.   II, III
    Vinyl Polymerization, Volume 1, Part I, edited by G. E. Ham
    (Marcel Dekker, Inc., New York, 1967)

Chapter 8: Heats of Polymerization and their Structural and Mechanistic Implications

The authors discuss experimental methods used to measure and derive enthalpies of poly-
merization. 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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43. Karapet'yants, M. Kh., and Karapet'yants, M. L.   II, II
    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", Moskva, 1968)

This book is a compilation of $\Delta H_f°$, $\Delta G_f°$, $S°$, 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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44. Kaufmann, D. W. (editor)   III, II
    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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45. Kazavchinskii, Ya. Z., Kessel'man, P. M., Kirillin, V. A.,   III, II
    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 Tyazhelaya 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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Keevan, H. J., Keyes, F. G., Hill, P. G., and Moore, J. G. -- see entry no. 99
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46. Kortum, G., Vogel, W., and Andrussow, K.   II, I
    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 coded in Part II, on use of the
table, where methods of calculation and corrections for solvent and for hydrolysis of salts
in conductivity measurements are also coded, for reference in the table. The Table itself
is arranged by acid class including: aliphatic and alicyclic carboxylic acids, aromatic
carboxylic acids, phenolic acids, and other acids and special classes. The Table gives the
name, chemical formula, and thermodynamic dissociation constant K of each acid, the tempera-
ture (°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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47. Krebs, H. A., and Kornberg, H. L., with appendix by K. Burton   I, II
    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

47. (continued)

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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48. Latimer, W. M. II, I
    The Oxidation States of the Elements and their Potentials in Aqueous Solution
    (second edition)
    (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1959)

This book contains extensive tables of $\Delta G_f°$, $\Delta H_f°$, and $S°$ values for the elements and their compounds as well as electrode potential diagrams calculated from the tabulated $\Delta G_f°$ values, from other measurements, and estimates when appropriate. Much of the tabulated data were taken from National Bureau of Standards Circular 500 (see entry no. 73). The appendixes include activity coefficient data for 77 strong electrolytes and a discussion of methods whereby entropies may be estimated.

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49. Lewis, G. N., and Randall, M. III, I
    (revised by Pitzer, K. S., and Brewer, L.)
    Thermodynamics
    (McGraw-Hill Book Company, New York, 1961)

This standard textbook on thermodynamics contains an Appendix of selected data for aqueous electrolyte solutions. Compiled are activity coefficients, relative partial molal enthalpies, and relative partial molal heat capacities for about 70 of the most common electrolytes in aqueous solution at 25 °C.

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50. Linke, W. F., and Seidell, A. II, I
    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, DC, 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. References are given to the data sources.

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51. Long, C. (editor)   I, II
    Biochemists Handbook
    (D. Van Nostrand Co., Princeton, New Jersey, 1961)

This reference book contains several tables of thermochemical data:

S. P. Datta and A. K. Grzybowski   pH and Acid-Base Equilibria

This chapter 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).

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K. Burton   Free Energy Data and Oxidation-Reduction
                                          Potentials

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

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52. Martell, A. E., and Smith R. M.   I, II
    Critical Stability Constants. Volume I: Amino Acids
    (Plenun Press, New York, 1974)
              and
    Smith, R. M., and Martell, A. E.
    Critical Stability Constants. Volume II: Amines
    (Plenum Press, New York, 1975)

Volume I contains selected values of log K, ΔH, and ΔS 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 arrangment of data is similar to that of the work of Sillen,
Martell, Hogfeldt, and Smith except that 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 II (415 pages) is similar in arrangement to Volume I. The organic ligands dealt with
are the aliphatic, secondary, and tertiary amines, azoles, azines, and the amino phosphorous
acids.

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53. Meites, L. (editor)   II, II
    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

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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53. (continued)

L. Meites   Formal Equilibrium Constants of Proton-transfer
                                             Reactions at Finite Ionic Strength

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, Chemical Society, London, 1957. Also
given are tables of acid dissociation data pertinent to ethanol-water and methanol-water
mixtures.

D. A. Aikens and C. N. Reilley   Formation Constants of Metal Complexes

Tabulated are log K values for the binding of the more common inorganic metal ions to 55
ligands. ΔH and ΔS values are also given for four ligands. Literature references are
given.

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54. Merrill, A. L., and Watt, B. K.   I, III
    Energy Value of Foods; Basis and Derivation
    Agriculture Handbook No. 74, 1955

    Watt, B. K., and Merill, A. L.
    Composition of Foods; Raw, Processed, Prepared
    Agriculture Handbook No. 8, revised, 1963

    (U. S. Government Printing Office, Washington, DC 20402)

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 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 1-5 and table 24 give enthalpies
of combustion of specific food items or component substances. Care should be used in
taking values from the numberous 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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55. Miller, D. G.   III, I
    Application of Irreversible Thermodynamics to Electrolyte Solutions. I. Determination of
    Ionic Transport Coefficients ℓ_{ij} for Isothermal Vector Transport Processes in Binary
    Electrolyte Systems. II. Ionic Coefficients ℓ_{ij} for Isothermal Vector Transport
    Processes in Ternary Systems.
    Journal of Physical Chemistry, 70, 2639 (1966); 71, 616 (1967)

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

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56. Millero, F. J. III, I
The Partial Molal Volumes of Electrolytes in Aqueous Solutions. Compilation
of the Partial Molal Volumes of Electrolytes at Infinite Dilution, $\overline{V}°$ and the Apparent
Molal Volume Concentration Dependence Constants, S_V^* and b_V, at Various Temperatures

Water and Aqueous Solutions, R. A. Horne (editor)
(Wiley-Interscience, New York, 1972)

This chapter is concerned with the measurement and interpretation of partial
molal volumes and their concentration and temperature dependences. Included are tables of
the partial molal volumes of the common inorganic and organic electrolytes (about 200
systems) as well as values of the partial molal volumes of the more common inorganic and
organic ions (about 100 species). The data refer to temperatures from 0 to 200 °C.

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57. Millero, F. J. · III, I
The Molal Volumes of Electrolytes
Chemical Reviews, 71, 147 (1971)

This is a detailed and thorough review article dealing with molal volumes of electrolytes
in water. Included is a history and discussion of theoretical developments associated with
molal volumes. Tabulated are the partial molal volumes of the common (about 50) inorganic
and organic ions in water at temperatures ranging from zero to 200 °C. There is also
given partial molal volume data for non-aqueous systems. There are 366 references to the
literature. Also see entry no. 56 above.

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58. Mishchenko, K. P., and Poltoratzkii, G. M. II, I
Aspects of the Thermodynamics and Structure of Aqueous and Non-Aqueous Electrolyte
Solutions
(Izd. "Khimia", Leningrad, 1968) (In Russian)

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 $\Delta H_f°$, $\Delta G_f°$, S and C_p
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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Naoomov, G. B., Rhizenko, B. N., and Kodakovski, I. L. -- see entry no. 100

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59. Parker, V. B.   III, I
    Thermal Properties of Aqueous Uni-univalent Electrolytes
    (NSRDS NBS 2, U. S. Government Printing Office, 1965)

This short (41 pp.) 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 dilute
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 molal
heat capacity and molal 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 for each
parameter and compound are arranged in a series of 21 tables for t = 25 °C.

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60. Parker, V. B., Wagman, D. D., and Garvin, D.   III, II
    Selected Thermochemical Data Compatible with the CODATA Recommendations
    (National Bureau of Standards Report No. 75-968, Washington, DC, 1976)

Selected thermochemical properties, $\Delta G_f°$, $\Delta H_f°$, $S°$, $Cp°$ (all at 298.15 K), $\Delta H_f°$ (0 K), and
H (298 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 CODATA Recommended Key Values for Thermodynamics).

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61. Parsons, R.   III, I
    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 molal 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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62. Pauling, L.   III, III
    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.

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63. Pedley, J. B. (editor)   III, II
    Computer Analysis of Thermochemical Data (CATCH Tables)
    (University of Sussex, Brighton, England, 1972 to present)

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. To date, the following tables have appeared:

Element	Author(s)	Year
Halogen Compounds (Fluorine, Chlorine, Bromine, Iodine)	J. D. Cox	1972
Nitrogen	G. Pilcher	1972
Phosphorous	A. J. Head	1972
Silicon	J. B. Pedley and B. S. Iseard	1972
Chromium, Molybdenum and Tungsten	D. S. Barnes	1974

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64. Perrin, D. D.   II, II
    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 217 compounds, preceded by a brief introduction to the use of the 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 extra-
polation to ionic strength $I = 0$. 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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65. Perrin, D. D.   II, II
    Dissociation Constants of Organic Bases in Aqueous Solution
    (Butterworths, London, 1965)

Published in the same series as the book by Kortum, Vogel, and Andrussow, this book tabulates
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.

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66. Phillips, R.   I, II
    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. Included for the tabulated data are the ionic strength,
temperature, supporting electrolyte, pH, method of measurement, and references to the
original data source.

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67. Phillips, R. C., George, P., and Rutman, R. J.   I, II
    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. A critical evaluation of the existing data pertinent
to this computation is included. References to 24 papers are given.

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68. Pourbaix, M. (and others)   III, I
    Atlas of Electrochemical Equilibrium in Aqueous Solution
    (Pergammon 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.

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69. Reid, R. C., and Sherwood, T. K.   III, II
    The Properties of Gases and Liquids, Their Estimation and Correlation (second edition)
    (McGraw-Hill Book Co., New York, 1966)

This lengthy monograph discusses various methods available for
calculating or 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
molal 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.

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70. Robinson, R. A., and Stokes, R. H.   II, I
    Electrolyte Solutions. The Measurement and Interpretation of Conductance, Chemical
    Potential and Diffusion in Solution of Simple Electrolytes (second edition, revised)
    (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°) 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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71. Rossini, F. D., Pitzer, K. S., Arnett, R. L., Brown, R. M., and   II, III
    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. 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. This is a revision of NBS Circular C461 (entry no. 72 below).

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

This monograph was prepared as part of the work of the American Petroleum Institute (API)
Research Project 44. Values are given for 36 physical and thermodynamic properties of
several hundred hydrocarbons in metric and in U. S. Customary units. The data in most
instances represent values found 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. Entry no. 71 above is a revision of this work.

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73. Rossini, F. D., Wagman, D. D., Evans, W. H., Levine, S., and   II, II
     Jaffe, I.
     Selected Values of Chemical Thermodynamic Properties
     National Bureau of Standards Circular 500 (1952)
     (U. S. Government Printing Office, Washington, DC 20402)

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
$\Delta H_f°_0$, $\Delta H_f°_{298}$, $\Delta G_f°_{298}$, log K_f, $S°_{298}$, and $C_p°_{298}$. 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 by competent thermochemists and
functions tabulated, maintaining internal consistency by the relationship:
$\Delta G_f°_{298} = \Delta H_f°_{298} - T\Delta S°_{298}$. The sources of data for each data item are listed and a
bibliography is included. Some information in this book can still not be found readily
elsewhere as the revision is not yet complete. Also, see Wagman, et al. in this
bibliography.

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74. Schafer, D., and Lax, E. (editors)   II, III
     Landolt-Börnstein
     Zahlenwerte und Fuctionen aus Physik, Chemie, Astronomie, Geophysik, und Technik,
     Sechste Auflage
     Eigenschaften der Materie in Ihren Aggregatzustanden
     4 Teil, Kalorische Zustandsgrossen
     (Springer-Verlag, Berlin, 1961) (in German)

This most recent issue of thermodynamic information of the Landolt-Bornstein series gives
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 kcal mol^{-1} and kJ 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.

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75. Sillen, L. G., Martell, A. E., Hogfeldt, E., and Smith, R. M.   II, I
     Stability Constants of Metal Ion Complexes, Section I: Inorganic Ligands,
     Section II: Organic Ligands (second edition)
     (Special Publication No. 17, The Chemical Society, London, England, 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 1961-63; the scope of the inorganic
section has been extended to cover redox equilibria and the extraction of inorganic
ligands into non-aqueous 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

75. (continued)

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; 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, β, 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_p – 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 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.

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76. Silvester, L. F., and Pitzer, K. S.   III, I
    Thermodynamics of Geothermal Brines. I. Thermodynamic Properties of Vapor Saturated
    NaCl (aq) Solutions from 0 to 300 °C
    (National Technical Information Service, Report No. LBL-4456, U. S. Department of Commerce,
    Springfield, VA)

Osmotic and activity coefficient data, enthalpy data, and heat capacity data on aqueous sodium chloride solutions covering the temperature range 0 to 300 °C were used to obtain the coefficients of an equation that could be used to predict these thermodynamic properties over the indicated temperature range. Tabulated are values of the total Gibbs energy, enthalpy, and heat capacity, partial molal and excess thermodynamic properties for sodium chloride in water from 0 to 300 °C and from 0 to 6 molal.

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77. Skinner, H. A. (editor)   III, II
    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:

Author(s)   Chapter

I. Wadsö   Biochemical Thermochemistry

R. F. Jameson   Thermodynamics of Metal-Complex Formation

77. (continued)

Author(s)	Chapter
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 latter article provides a very useful guide to much of the evaluated thermodynamic data that is not covered in this bibliography.

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Smith, R. M., and Martel, R. E. -- see entry no. 52

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78. Sober, H. A. (editor)   I, II
    Handbook of Biochemistry - Selected Data for Molecular Biology
    (The Chemical Rubber Co., Cleveland, 1968) (see also second edition, 1970)

This compendium contains the following twenty-three tables of thermochemical data. The same tables, some containing additional information are in the second edition (indicated in parentheses).

Author or Source	Table
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

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

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J. O. Hutchens	Heat Capacities, Absolute Entropies, and Entropies of Formation of Amino Acids and Related Compounds

Cp°, S°, and ΔS_f° at 25 °C are tabulated for 28 amino acids, 3 peptides, 4 proteins, and 3 related substances.

J. O. Hutchens and E. P. Kirby Hade, Jr.	Solubilities of Amino Acids in Water at Various Temperatures

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

J. O. Hutchens	Heats of Combustion, Enthalpy and Free Energy of Formation of Amino Acids and Related Compounds

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

J. O. Hutchens	Heats of Solution of Amino Acids in Aqueous Solution at 25 °C

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

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78. (continued)

<table>
<tr><td>Author or Source</td><td>Table</td></tr>
<tr><td>J. O. Hutchens</td><td>Free Energies of Solution and Standard Free Energies of Formation of Amino Acids in Aqueous Solution at 25 °C</td></tr>
</table>

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

J. O. Hutchens   Activities of Amino Acids and Peptides at 25 °C

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

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

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

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

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

From K. S. Markley, "Fatty Acids. Part I", second edition, Interscience, New York (1960)   Solubilities of Simple Saturated Triglycerides

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

From K. S. Markley, "Fatty Acids. Part I", second edition Interscience, New York (1960)   Solubilities of Mixed Triacid Triglycerides at 25 °C

Tabulated are solubilities of four mixed triacid triglycerides in four non-aqueous solvents.

P. A. Loach   Oxidation-Reduction Potentials, Absorbance Bands in Biochemical Studies

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

R. W. Henderson and T. C. Morton   Oxidation-Reduction Potentials of Hemoproteins and Metalloporphyrins

Tabulated are oxidation-reduction potentials for 241 (282) hemoproteins and metalloporphyrins at assorted temperatures.

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78. (continued)

<u>Author or Source</u>   <u>Table</u>

R. M. Izatt and J. J. Christensen   Heats of Proton Ionization and Related
                                                    Thermodynamic Quantities

This section is an extensive tabulation of enthalpy and entropy changes and pK values for
organic and biochemical systems with 323 (418) references to the literature.

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G. C. Krescheck   Calorimeteric ΔH Values Accompanying Conforma-
                                                    tional Changes of Macromolecules in Solution

Tabulated are ΔH values accompanying the conformation changes of 25 macromolecular systems.

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W. P. Jencks   Free Energies of Hydrolysis and Decarboxylation

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

Given is an extensive tabulation of pK values for ionization of several hundred acids and
bases with 116 (117) references to the literature.

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R. G. Bates   Measurement of pH
R. G. Bates   Buffer Solutions

pH values have been assigned to several important buffer systems.

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Good, Winget, Winter, Connolly,   Properties of Some New Buffers for Biological
 Izawa, and Singh, Biochemistry,   Research
 <u>5</u>, 472 (1966)

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

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79. Stephen, H., and Stephen, T.   II, I
     Solubilities of Inorganic and Organic Compounds (in five volumes)
     (Pergammon Press, Oxford, 1963)

This series of five volumes (about 5500 pages) 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.

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80. Stull, D. R., Westrum, E. F., and Sinke, G. C.   II, III
     The Chemical Thermodynamics of Organic Compounds
     (John Wiley and Sons, Inc., New York, 1969)

This monograph is divided into three parts. The first part gives 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 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 $C_p°$, $S°$, $-(G - H°_{298})/T$, $H°$, $H°_{298}$, $\Delta H_f°$, $\Delta G_f°$, and log K_p are given
at 100 K intervals. In the third section are listed selected values of enthalpy of
formation, entropy, and consistent values of $\Delta G_f°$ and log K_p of organic compounds at 298 K.
In excess of 4000 compounds are listed. A very few inorganic compounds are also found in
this book. A chapter very briefly discusses methods of estimating thermodynamic quantities.

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81. Tatevskii, V. M., Benderskii, V. A., and Yarovoi, S. S.   III, III
     Rules and Methods for Calculating the Physico-Chemical Properties of Paraffinic
     Hydrocarbons

     (Pergamon Press, New York, Oxford, London, Paris, 1961)
     Translated from the Russian Zakonomernosti i metody rascheta fiziko-khimicheskikh
     svoistv parafinovykh 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. It suffers from ambiguity of statement which is somewhat distracting, but the
methods presented in it have been attracting increasing attention recently. 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.

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82. Timmermans, J.   II, III
     Physico-Chemical Constants of Pure Organic Compounds (in two volumes)
     (Elsevier Publishing Co., Amsterdam, 1950 and 1965)

These two volumes contain tables of physical data for pure organic compounds. The arrange-
ment 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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83. Timmermans, J.   II, II
     The Physico-Chemical Constants of Binary Systems in Concentrated Solutions
     (in four volumes)
     (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

83. (continued)

properties. This reference contains 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.

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Travers, J. G., Dellieu, I., and Hepler, L. G. -- see entry no. 102

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84. Wagman, D. D., Evans, W. H., Parker, V. B., and (in various individual   II, II
 parts) Halow, I., Bailey, S. M., Schumm, R. H., Churney, K. L.
 Selected Values of Chemical Thermodynamic Properties
 National Bureau of Standards Technical Note 270, October 1965 (and continuing)
 (U. S. Government Printing Office, Washington, DC 20402)

This technical note is a revision of NBS Circular 500 Part I (see above) and is issued in parts as segments of the work relating to selected sequences of elements are completed. The following parts had been issued as of 1974.

270-1   Tables for the first twenty-three elements in the standard order of arrangement.

270-2   Tables for elements 24-32 in the standard order of arrangement.

270-3   Tables for the first thirty-four elements in the standard order of arrangement. This table includes thermochemical data for compounds containing one or two carbon atoms. This technical note supersedes technical notes 270-1 and 270-2.

270-4   Tables for elements 35-53 in the standard order of arrangement.

270-5   Tables for elements 54-61 in the standard order of arrangement.

270-6   Tables for the alkaline earth elements, elements 92-97 in the standard order of arrangement.

270-7   Tables for the Lanthanide (Rare Earth) elements, elements 62-76 in the standard order of arrangement.

The remaining elements are to be covered in two or three additional parts to appear over a period of about two years. Documentation and references have not yet been issued.

This is the most comprehensive recent compilation in English of critically evaluated 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 any of the properties tabulated. The coverage when complete will be approximately 12,000 substances. Properties tabulated are $\Delta H_f^{\circ}{}_0$, $\Delta H_f^{\circ}{}_{298}$, $\Delta G_f^{\circ}{}_{298}$, $H^{\circ}{}_{298.15} - H^{\circ}{}_0$, $S^{\circ}{}_{298}$, $C_p^{\circ}{}_{298.15}$. The data from original sources have been critically evaluated by competent thermochemists and "best" values selected for the functions tabulated, maintaining internal consistency by the relationships $\Delta G_f^{\circ}{}_{298} = \Delta H_f^{\circ}{}_{298} - T\Delta S_f^{\circ}{}_{298}$, and $\Delta H_f^{\circ}{}_{298} - \Delta H_f^{\circ}{}_0 = \Sigma(H^{\circ}{}_{298} - H^{\circ}{}_0)$.

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

This large (seven volume) but largely superseded compendium of information contains still
valid tables of thermodynamic data as well as useful 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.

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86. Westrum, E. F. (editor)   III, I
    Bulletin of Thermodynamics and Thermochemistry
    (University of Michigan, Ann Arbor, Michigan)

The 18th annual issue appeared in 1975. The Bulletin is a current awareness bibliography
of articles that pertain to thermodynamics and thermochemistry. The Bulletin is presently
divided into sections on inorganic systems, organic systems, organic systems (mixtures),
and, since 1971, biological and macromolecular systems. Also included are sections on work
in progress at various laboratories, substance-property indexes, and bibliographies on
books of interest to thermodynamicists. No data values are given. Prior to the issuance
of the Bulletin, the yearly volumes of the Annual Reviews of Physical Chemistry, published
since 1950 by Annual Reviews, Inc., Palo Alto, California, usually contained bibliographic
information dealing with general thermochemistry and the thermodynamics of electrolyte
solutions. These articles were the forerunners of the Bulletin of Thermodynamics and
Thermochemistry.

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87. Wilhelm, E., and Battino, R.   III, I
    Thermodynamic Functions of the Solubilities of Gases in Liquids at 25 °C
    Chemical Reviews, $\underline{73}$, 1 (1973)

This review article contains selected values for the solubility, entropy, and enthalpy
changes on 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.

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88. Wilhoit, R. C., and Zwolinski, B. J.   II, III
    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 subject data on 680 hydrocarbons, 95 sulfur compounds, and water from
0 to 150 °C. It is indexed by compound name, and by boiling point.

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89. Wilhoit, R. C., and Zwolinski, B. J.   III, III
    Physical and Thermodynamic Properties of Aliphatic Alcohols
    Journal of Physical and Chemical Reference Data, $\underline{2}$ (Supplement No. 1), 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.

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90. Wu, Y. C., and Hamer, W. J.   III, I
    Electrochemical Data. Part XIV. Osmotic Coefficients and Mean Activity Coefficients
    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
    (National Bureau of Standards Reports No. 10052 and 10088, U. S. Department of Commerce,
    1969)

These reports give values for the osmotic and mean activity coefficients of uni-bivalent,
vi-univalent, 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.

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91. Yatsimirskii, K. B., and Vasil'ev, V. P.   II, II
    Instability Constants of Complex Compounds
    (Consultants Bureau, New York, 1966) and
    (Pergammon 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.

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92. Zordan, T. A., and Hepler, L. G.   III, II
    Thermochemistry and Oxidation Potentials of Manganese and Its Compounds
    Chemical Reviews, $\underline{68}$, 737 (1968)

This review contains selected values of $\Delta G_f°$, $\Delta H_f°$, $S°$, and electrochemical potentials for
manganese and about 45 of its inorganic compounds and aqueous species at 25 °C. Included
are the more important aqueous species and references to the primary literature.

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93. Baes, C. F., Jr., and Mesmer, R. E.   III, I
     The Hydrolysis of Cations
     (John Wiley & 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, ΔH
and ΔS data for the hydrolysis reactions are also presented. The data, with references and
comments, is arranged under the element of interest.

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94. Bates, R. G.   II, II
     Determination of pH, Theory and Practice (Second Edition)
     (John Wiley & 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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95. Boublik, T., Fried, V., and Hala, E.   II, III
     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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96. Gedansky, L. M., Woolley, E. M., and Hepler, L. G.   III, II
     Thermochemistry of Compounds and Aqueous Ions of Copper
     Journal of Chemical Thermodynamics 2, 561 (1970)

This article is a critical review and selection of thermochemical data for the element copper
and about 90 of its compounds and aqueous species. Tabulated are selected values of
$\Delta H_f°$, $\Delta G_f°$, $S°$ and electrode potentials at 25 °C. There are 89 references to the primary
literature.

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97. Ingraham, L. L., and Pardee, A. B.   I, III
     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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98. Jazimirski (Yatsimirskii), K. B.   III, II
     Thermochemie von Komplexverbindungen
     (Akademie-Verlag, Berlin, 1956) translated from the Russian by Georg Crull
     Thermochimia Complexnik Coedinenie
     (AKAD NAUK CCCP, MOCKVA 1951)

This monograph correlates 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.

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99. Keenan, H. J., Keyes, F. G., Hill, P. G., and Moore, J. G.   III, II
     Steam Tables – Thermodynamic Properties of Water, Including Vapor, Liquid, and
     Solid Phases (International Edition, Metric Units)
     (John Wiley & Sons, New York, 1969)

This book presents the results of a new and independent correlation of the thermodynamic
data for water. It is a complete revision of 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.

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100. Naoomov, G. B., Rhizhenko, B. N., and Kodakovskii, I. L.   III, II
     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
$\Delta G_f°$, $\Delta H_f°$, $S°$, and $C_p°$ at 298 K; electrode potentials; enthalpies and entropies for phase
transitions; $\Delta G_f°$ of inorganic aqueous ions from 25 to 350 °C; partial molal heat capacities
from 10 to 130 °C; and the partial molal 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.

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101. Stull, D. R.   II, III
     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 compound has a
given vapor pressure.

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102. Travers, J. G., Dellieu, I., and Hepler, L. G.   III, II
     Scandium: Thermodynamic Properties, Chemical Equilibria, and Standard Potentials
     Thermochimica Acta 15, 89 (1976)

This article is a critical review and selection of thermochemical data for the element
scandium and its compounds including aqueous species. Tabulated are selected values of
$\Delta H_f°$, $\Delta G_f°$, $S°$ and electrode potentials at 25 °C. There are 79 references to the primary
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16. ABSTRACT *(A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here.)*

Contained herein 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 molal 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.

17. KEY WORDS *(six to twelve entries; alphabetical order; capitalize only the first letter of the first key word unless a proper name; separated by semicolons)* Aqueous systems; bibliography; biochemical systems; enthalpy data; entropy data; equilibrium data; Gibbs energy data; heat capacity data; partial molal properties; thermochemistry; thermodynamics; review articles; water pollution.

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