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NIST-JANAF Thermochemical Tables Fourth Edition Part I, Al-Co

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Foreword

The Journal of Physical and Chemical Reference Data is published jointly by the American Institute of Physics and the American Chemical Society for the National Institute of Standards and Technology. Its objective is to provide critically evaluated physical and chemical property data, fully documented as to the original sources and the criteria used for evaluation. One of the principal sources of material for the journal is the National Standard Reference Data System (NSRDS), a program coordinated by NIST for the purpose of promoting the compilation and critical evaluation of property data.

The regular issues of the Journal of Physical and Chemical Reference Data are published bimonthly and contain compilations and critical data reviews of moderate length. Longer works, volumes of collected tables, and other material unsuited to a periodical format have previously been published as Supplements to the Journal. In 1989 the generic title of these works was changed to Monograph, reflecting their character as independent publications.

This volume, the Fourth Edition of the NIST-JANAF Thermochemical Tables, is Monograph No. 9 in the current series. Its predecessor, the Third Edition, was referred to as a Supplement. Of the over 500 titles published in the last 25 years, the articles dealing with the JANAF Thermochemical Tables have been the most widely distributed and used.

The Journal of Physical and Chemical Reference Data is therefore pleased to be able to publish this Fourth Edition of the NIST-JANAF Thermochemical Tables. There are two important features of this edition. First, the acronym NIST has been added to the title of this activity. This is due to the fact that during the past 10 years, NIST has been the leading financial supporter for this effort. Additionally, this project is now housed within the Physical and Chemical Properties Division at NIST. Second, the Fourth Edition contains additional species not included in the Third Edition. A number of typographical errors have also been corrected.

Malcolm W. Chase, Jr., Editor
Journal of Physical and Chemical Reference Data

Preface to the First Edition

Beginning in the mid-1950s, when elements other that the conventional carbon, hydrogen, oxygen, nitrogen, chlorine, and fluorine came into consideration as rocket propellant ingredients, formidable difficulties were encountered in conducting rigorous theoretical performance calculations for these new propellants. The first major problem was the calculational technique. The second was the lack of accurate thermodynamic data.

By the end of 1959, the calculational technique problem had been substantially resolved by applying the method of minimization of free energy to large, high speed digital computers. At this point the calculations became as accurate as the thermodynamic data upon which they were based. However, serious gaps were present in the available data. For propellant ingredients, only the standard heat of formation is required to conduct a performance calculation. However, this must be known to a high degree of accuracy. For combustion products, the enthalpy and entropy must be known, as a function of temperature, in addition to the standard heat of formation.

In order to resolve the problem, a substantial experimental thermodynamic research program was initiated under the sponsorship and technical direction of Project PRINCIPIA of the Advanced Research Projects Agency. Simultaneously, a project was initiated to critically evaluate and compile consistent tables of thermodynamic properties of propellant combustion products for use by the aerospace industry. This project, known as the JANAF Thermochemical Tables, was undertaken by the Dow Chemical Company. Since the objective of the project was to have one single source of best available data prepared for use by the entire industry, the JANAF Thermochemical Panel undertook the task of furnishing a critical review of the Tables prior to their publication and distribution. This approach was designed to ensure that the Tables be of the highest possible quality.

Washington, DC
July 1964

C. V. Mock
Advance Research Projects Agency

Preface to the Second Edition

It is appropriate to call attention to some of the reasons for the phenomenal success of the JANAF Thermochemical Tables in achieving, first, the initial limited objective of providing the standard data for the chemical rocket propulsion industry, and later, upon publication, worldwide recognition as thermodynamic reference data of the highest quality and timeliness.

First, and most obvious, there was the selection and continued support of a highly competent evaluation team, themselves engaged in a broad spectrum of thermodynamic research. The personnel of the Thermal Research Laboratory of the Dow Chemical Company, under the direction of Dr. D. R. Stull and Dr. H. Prophet, have filled this role to a degree of excellence not likely to be exceeded anywhere. Moreover, the group has heroically remained productive in spite of many battles to retain continuing support, and the actual sharp reduction of funding over the past two years to a less-than-viable level.

A second important factor is the unusual approach to format, evaluation, and distribution of the Tables, as it has been followed since their inception. The primary distribution is in frequently issued loose-leaf supplements. Each previously issued table may thus be revised as often as necessary to take account of improved data. Each loose-leaf table is accompanied on its reverse side by a complete explanation of the selection of the key data, together with all references.

The third vital distinction of these tables has been the existence of a continuing cognizant working group composed of technological users of data, thermodynamicists, and government sponsors of both research and development. Independent prepublication review of the Tables has been an important contribution of some of the members of this group; but its annual technical meetings have resulted in even more far-reaching benefits. Together, the users and generators of data have been able to establish realistic priorities for the species to be included in the Tables; at the same time the course of experimental research has been guided by the demonstration of absence or inadequacy of needed data. Although the working group no longer enjoys official recognition, the members and participants have enthusiastically volunteered to continue meeting in this important work.

Special words of appreciation are due to Dr. Charles W. Beckett, who has lined up all the technical presentations at the last six annual meetings of the working group; and to Mr. Curtis C. Selph who has served with wisdom and insight as the Air Force project monitor for the JANAF Thermochemical Tables contracts.

Arlington, Virginia
October 1970

Joseph F. Masi
Air Force Office of Scientifc Research

Preface to the Third Edition

The United States Air Force (USAF) for more than 20 years has supported, and continues to support, the preparation of the JANAF Thermochemical Tables. The Tables, funded through Air Force Office of Scientific Research (AFOSR), were intended originally for calculating performance of thermochemical reactors, such as rocket engines. The computation of such performance figures as thrust and exhaust temperature for a rocket require data such as those in these tables.

The Department of Energy (DOE) [and predecessor agencies Energy Research and Development Administration (ERDA), Office of Coal Research, and Bureau of Mines] became interested in the JANAF Thermochemical Tables because the tables had become *the* benchmark for thermochemical data for performance calculations. However, reactors and reagents of interest to DOE are different from those of the USAF.

The Department of Energy needs performance calculations for several types of reactors that are of interest in fossil fuel research. These reactors include air pollution control equipment, automotive internal combustion engines, coal gasifiers and furnaces, fuel cells, liquefaction reactors and their catalyst structures, and magnetohydrodynamic generators. For example, researchers might wish to calculate the first-law efficiency of an electrical power plant, or the exhaust concentration of a pollutant such as sulfur dioxide or mercury.

The calculations needed for DOE interests have as their basis the same mathematics and physical chemistry as required for the performance calculations of USAF interest, but DOE needs tables for more and different chemicals. For example, a rocket fuel probably would not be formulated to include silicon or sulfur, but all known coals contain both these elements. Silicon and sulfur are two distinguishing elements accounting for many peculiarities of coal utilization chemistry (which include the chemistries of all the polysulfides, thiosulfates, alums, etc., and of the many glasses and mixed silicates).

For more than six years (1975-1982), Dow Chemical has worked on separate but complementary contracts to satisfy the thermochemical tables' needs of USAF and DOE. This Third Edition of the JANAF Thermochemical Tables presents the results of these efforts, along with reformatted versions of previous tables, to provide an extensive set of tables of wide utility that are consistent with each other and with the requirements of thermodynamic theory.

There remain open questions about calculation methods for equilibrium problems. I mention this because the foreword for the First Edition endorses free-energy-minimization as if it solved all problems of numerical instability. I would remove this apparent endorsement as confusing, inappropriate, and uninformative for users of these tables. For example, the paper of White, Johnson, and Dantzig [J. Phys. Chem. 28, 751 (1958)] does not address numeric stability in any way. Removing this endorsement would not diminish Dow's JANAF work.

I want to thank several people. All the Dow personnel did outstanding work, and several fellow federal employees helped with orchestrating the various contracts to nourish this finished product. In AFOSR, Joseph Masi, Robert Sperlein, and Leonard Caveny were always encouraging. Within the Bureau of Mines, then in ERDA, and finally in DOE, I was helped and encouraged by Daniel Bienstock, Irving Wender, Jim Hendrie, Alex Mills, Kermit Woodcock, and Mike Hogan.

Pittsburgh, Pennsylvania
April 1984

Francis E. Spencer, Jr.
Pittsburgh Energy Technology Center
Department of Energy

Preface to the Fourth Edition

As the Standard Reference Data Program at the National Institute of Standards and Technology approaches its thirtieth year, the release of the fourth edition of the NIST-JANAF Thermochemical Tables provides not only a major update to this important reference work, but also a symbol of the long-term dedication of NIST and its scientists to improving the quality and accessibility of scientific data.

First, let us address the importance of the NIST-JANAF Thermochemical Tables. This fourth edition continues to serve its original community, that is, the scientists and engineers who design rocket propellants. For this use, the updated tables offer additional species and in some cases, corrected data for older species. The use of the NIST-JANAF Thermochemical Tables, however, now far transcends the original need. Today, as modeling of complex chemical processes is becoming routine, NIST-JANAF information is an invaluable resource for reliable thermochemical data. Care of preparation and critical evaluation still form the essence of the compilation. New users are demanding new species, and the tables are being responsive to those demands. There is no other comprehensive source of temperature dependent thermochemical data for inorganic species, certainly none of such high quality.

From another perspective, this edition is an important milestone, for this publication again demonstrates the long-term commitment by NIST to providing evaluated scientific and technical data through its Standard Reference Data Program. Established by the Standard Reference Data Act of 1968, the program today operates data evaluation activities in most areas of NIST's scientific and engineering work.

The Physical and Chemical Properties Division of the NIST Chemical Science and Technology Laboratory (and its predecessors) has for many decades been committed to providing critically evaluated thermochemical data. The "International Critical Tables," "The NIST Tables of Chemical Thermodynamic Properties; Selected Values for Inorganic and C_1 and C_2 Organic Substances in SI Units," and now the "NIST-JANAF Thermochemical Tables" are prime examples of the fruit of this commitment.

The scientific effort required to produce critically evaluated data is difficult for the non-specialist to appreciate. Even though many thermochemical, experimental, and theoretical techniques are well-developed, rarely does one individual measurement or calculation provide "property data." Instead most properties of substances come from repeated measurements, done over time and by different groups, and it is the job of the data evaluator to reconcile conflicting information and extract standard reference data of the type presented in the NIST-JANAF Thermochemical Tables. Malcolm W. Chase was the responsible scientist for the third and fourth editions, and the high quality of data contained in this latest edition is a tribute to his experience and skills as an evaluator.

Finally, it should be noted that the change of name to the NIST-JANAF Thermochemical Tables is the result of greater involvement by NIST in supporting the new edition. Data work at NIST is a team effort, in this case, of the Physical and Chemical Properties Division and the Standard Reference Data Program. The NIST-JANAF Thermochemical Tables represent a renewed dedication on the part of both organizations to make sure that scientists and engineers in industry, government, and academe have access to numeric recommendations of known reliability, for use in research, development, and related technical activities. NIST is proud to present this data compilation to the technical community.

Gaithersburg, Maryland
January 1998

Richard F. Kayser
Chief, Physical and Chemical Properties Division
and
John R. Rumble
Chief, Standard Reference Data Program

Contents

The Table of Contents is a cumulative listing of Parts I and II.
Part I contains pp. I-XI and 1–957 (Tables for Al-Co), and
Part II contains pp. 959–1951 (Tables for Cr-Zr).

1. Introduction

The Fourth Edition to the NIST-JANAF Thermochemical Tables has been assembled under the sponsorship of the Standard Reference Data Program at the National Institute of Standards and Technology. It contains tables of recommended temperature-dependent values for the standard enthalpy of formation, Gibbs (free) energy of formation, the logarithm of the equilibrium constant of formation, the heat capacity, entropy, enthalpy, and Gibbs energy function for 48 elements and many of their compounds. This publication is a current collection of all tables issued through 1997 under contracts with the U.S. Department of Energy and the U.S. Air Force Office of Scientific Research, NASA, the JANNAF Combustion Subcommittee, and the Standard Reference Data Program. It supersedes the Third Edition,[1] which, in turn, superseded the Second Edition,[2] and the four supplemental updates published in the Journal of Physical and Chemical Reference Data.[3–6]

Numerous new and revised thermochemical tables are included in this collection. [Refer to Sec. 7] Unlike the Third Edition of these tables, the Fourth Edition is not a rewriting and a recalculation of all the tables; no attempt has been made to reanalyze the data for all tables. A continued effort was made to correct all typographical errors from previous publications and to force an increasingly consistent style and format. The tables adhere more closely to the current IUPAC recommendations on symbols and notation. The tables, as published in the previous Third Edition, are all based on the 1981 IUPAC[7a] and 1973 CODATA[8a] recommendations for relative molecular masses and fundamental constants. As a result, a comparison of a table in the Fourth and Third Editions and their previously published form (i.e., same revision date) will reveal differences; however, these result from the adjustments mentioned above rather than from a reanalysis of the data. For tables issued since the Third Edition, values of the fundamental constants and relative molecular masses are based on the 1993 IUPAC[7b] and 1986 CODATA[8b] recommendations. It should be noted that there is a revised set of recommendations for the fundamental constants due in late 1998. Also, it should be remembered that the relative molecular masses are reassessed and updated every two years. The effects of these changes will be discussed later.

All thermal functions have been calculated using the same auxiliary data. Following a similar procedure for the formation properties has introduced slight inconsistencies in those tables for which the formation properties were derived from the previous thermal functions.

2. History of the JANAF Thermochemical Tables

Between 1955 and 1958, severe difficulties were encountered by individuals attempting to conduct rigorous performance calculations for propellant systems that gave multiphase combustion products characterized by complex chemical and thermal equilibria. Several of these individuals approached the Armed Services requesting that a group be assembled to assess the validity of the calculation methods and thermochemical data which were being employed at that time.

January 1958, the Armed Services jointly instructed the Solid Propellant Information Agency to organize the Joint Army-Navy-Air Force Ad Hoc Panel on Performance Calculation Methods and Thermodynamic Data. This panel, which consisted of 38 representatives of military facilities, defense contractors, and research organizations, terminated its operations in June 1959, with a recommendation that future activities under its purview could more appropriately be handled by a smaller working group. An additional recommendation included in the panel's final report was that this working group initiate the establishment of a thermochemical data compilation, evaluation, and dissemination program utilizing the available personnel and facilities of the Dow Chemical Company.

On 1 September 1959, the Joint Army-Navy-Air Force Thermochemical Panel was formed under the sponsorship of the Bureau of Naval Weapons, Department of the Navy; Office, Chief of Ordnance, Department of the Army; Air Research and Development Command, Department of the Air Force; and the Advanced Research Projects Agency, Department of Defense. The panel operated in accordance with the Rules of Operations of Solid Propellant Panels as adopted by representatives of the above offices on 1 September 1959.

The JANAF Thermochemical Panel Membership, which consisted originally of approximately 15 individuals with special experience in the technological subject under panel purview, met at the Pentagon on 16 November 1959, at which time plans for the thermochemical compilation project were reviewed and the project formally initiated.

Urgency required that a large set of consistent tables be assembled as quickly as possible. Computer programs had to be developed, and at first it was not possible to adequately assess the input information for every table. When the original data were evaluated, the table was printed on white paper; otherwise, the table was printed on gray paper. By the end of 1960, the first set was ready for distribution to some 1000 qualified recipients. For a number of years, at the end of each quarter, a supplement was issued which contained additional tables and revised tables. Some of the gray tables were revised to white tables.

The distribution of quarterly supplements continued through 31 December 1967, at which time the distribution shifted to semiannual supplements. Simultaneously, the tables were prepared under the auspices of the Interagency Chemical Rocket Propulsion Group, Working Group on Thermochemistry. On 31 December 1970, the working group became the Ad Hoc Working Group on Thermochemistry. By 30 June 1971, the tables project was sponsored by the U. S. Air Force Office of Scientific Research (AFOSR) and prepared under the advice and assistance of a thermochemistry group, referred to as reviewers. In late 1976, the U.S. Energy Research and Development Administration (now reorganized to be the U.S. Department of Energy) joined in sponsoring the tables.

The distribution reverted to a quarterly schedule with an expanded list of reviewers. AFOSR and DOE jointly funded this activity until late 1982. AFOSR continued as the sole sponsor until 1986.

From 1967 through 1985, the JANAF Thermochemical Tables have been sponsored by the U.S. Air Force Office of Scientific Research and the U.S. Department of Energy under the following contracts:

Air Force Contracts	Department of Energy Contracts
F04611-67-C-0009	DE AC22-76ET10637
F04611-70-C-0028	DE AC22-81PC41514
F44620-70-C-0104	
F44620-75-C-0048	
F49620-82-C-0016	

In addition, there was an interagency transfer of funds, from AFOSR to DOE, in the period 1976-1981.

In 1970 the output of the JANAF project was incorporated into the National Standard Reference Data System, a national program on evaluated physical and chemical data which is coordinated by the National Institute of Standards and Technology. Since that time the JANAF Thermochemical Tables have been disseminated as part of the Journal of Physical and Chemical Reference Data. Loose-leaf supplements were terminated with the publication of the Third Edition.

In January 1986, the JANAF Thermochemical Tables project transferred from the Dow Chemical Company to the National Institute of Standards and Technology. Funding since 1986 has come in large part from the Standard Reference Data Program, with additional contracts with NASA, JANNAF Combustion Subcommittee, and the U. S. Army. Updates to this Fourth Edition are being made in separate articles, many of which (but not all) are to be published in the Journal of Physical and Chemical Reference Data.

2.1. Members of the JANAF Thermochemical Panel (1959-1961) and the JANAF Thermochemical Working Group (1961-1964)

T. O. Dobbins, Advanced Research Projects Agency (Past Chairman)

W. H. Jones, Institute for Defense Analyses; Aerospace Corporation (Past Chairman)

W. G. May, Institute for Defense Analyses; Esso Research and Engineering Company (Past Chairman)

C. W. Beckett, National Bureau of Standards (Vice Chairman)

G. W. Avery, Chemical Propulsion Information Agency (Past Secretary)

B. K. Farris, Chemical Propulsion Information Agency (Past Secretary)

T. L. Reedy, Chemical Propulsion Information Agency (Secretary)

B. J. Alley, Army Materiel Command

P. W. Bender, University of Wisconsin

W. A. Bernett, Bureau of Naval Weapons

B. Brown, Hercules Powder Company

C. L. Funk, Jet Propulsion Laboratory

J. S. Gordon, Thiokol Chemical Corporation

L. J. Gordon, Aerojet-General Corporation

S. A. Greene, North American Aviation

C. B. Henderson, Atlantic Research Corporation

D. L. Hildenbrand, Philco Corporation

J. L. Margrave, University of Wisconsin

J. P. McCullough, U.S. Bureau of Mines

P. L. Nichols, Jr., Jet Propulsion Laboratory

C. C. Selph, Air Force Systems Command

D. R. Stull, Dow Chemical Company

The Thermochemical Working Group of the Interagency Chemical Rocket Propulsion Group (ICRPG) has consisted of the following at various times during its existence (1964-1969).

Members

J. F. Masi, Air Force Office of Scientific Research (Chairman)

C. W. Beckett, National Bureau of Standards (Vice Chairman)

T. O. Dobbins, Advanced Research Projects Agency

S. Gordon, National Aeronautics and Space Administration

R. Jackel, Office of Naval Research

J. Murrin, Naval Ordnance Systems Command

R. Odom, Army Materiel Command

C. C. Selph, Air Force Rocket Propulsion Laboratory

D. Squire, Army Research Office

Participants

G. S. Bahn, Marquardt Corporation

B. Brown, Hercules, Inc.

H. F. Calcote, AeroChem Research Laboratories

J. P. Coughlin, Aerojet-General Corporation

J. S. Gordon, Atlantic Research Corporation

D. R. Douslin, U.S. Bureau of Mines

M. Farber, Space Sciences, Inc.

R. M. Fristrom, Applied Physics Laboratory

C. B. Henderson, Atlantic Research Corporation

D. L. Hildenbrand, Douglas Aircraft Company

J. L. Margrave, Rice University

W. G. May, Esso Research and Engineering Company

W. Mitchell, Thiokol Chemical Corporation

C. F. Robillard, Jet Propulsion Laboratory

L. Schieler, Aerospace Corporation

C. H. Shomate, Naval Weapons Center

D. R. Stull, Dow Chemical Company

M. Zimmer, Naval Ordnance Station

Secretariat (Chemical Propulsion Information Agency)

T. Gilliland

M. McCormack

T. L. Reedy

In the period 1969-1984, various scientists donated their time to critique the loose-leaf supplements to the JANAF

Thermochemical Tables prior to their distribution. Their efforts certainly increased the quality of the tables. As of January 1982 the reviewers of the JANAF Thermochemical Tables were:

DOE Reviewers

Francis E. Spencer, Jr., DOE/PETC Combustion Technical Division
Joseph W. Martin, DOE/METC, Coal Projects Management Division
Thomas C. Ehlert, Marquette University
R. Howald, Montana State University
Fred C. Fehsenfeld, NOAA Environmental Research Laboratory
Gerd Rosenblatt, Los Alamos National Laboratory
Martin Steinberg, University of California, Santa Barbara
C. B. Alcock, University of Toronto
J. Brian Pedley, University of Sussex
Malcolm H. Rand, AERE Harwell.

AFOSR Reviewers

David White, University of Pennsylvania
W. L. Worrell, University of Pennsylvania
Stanley Abramowitz, U.S. National Bureau of Standards
David A. Ditmars, U.S. National Bureau of Standards
H. M. Rosenstock, U.S. National Bureau of Standards
Leonard Caveny, AFOSR/NA, Bolling AFB
John L. Haas, Jr., U.S. Geological Survey
John S. Gordon, TRW Energy Systems
Joseph F. Masi, AFOSR (retired)
Sanford Gordon, NASA Lewis Research Center
Edgar F. Westrum, Jr., University of Michigan
William D. Good, DOE/BETC
R. H. Hauge, Rice University
John L. Margrave, Rice University
Milton Farber, Space Sciences, Inc.
Curtis C. Selph, AFRPL/LKDH
Donald L. Hildenbrand, SRI International
Leo Brewer, University of California
James P. Coughlin, Aerojet Tactical Systems Co.
N. A. Gokcen, U.S. Bureau of Mines, AMRC

2.2. Project Personnel

The Tables began under the direction of Daniel R. Stull in 1959. Major contributions in the first two years were made by Thomas E. Dergazarian, Samuel Levine, and Louis A. DuPlessis. In 1969 Harold Prophet succeeded Daniel R. Stull as project director and continued in that position until his untimely death in late 1972. Malcolm W. Chase has been project director since late 1972.

The following professional personnel of the Dow Chemical Company have been involved in the preparation of the JANAF Thermochemical Tables:

Project Director, D. R. Stull	1959-1969
Project Director, H. Prophet	1969-1972
Project Director, M. W. Chase	1972-1985
P. A. Andreozzi	1980-83
J. Chao	1961-69
J. L. Curnutt	1969-79
T. E. Dergazarian	1959-63
C. A. Davies	1980-85
J. R. Downey, Jr.	1976-85
L. A. DuPlessis	1960-61
D. J. Frurip	1983-85
S. T. Hadden	1962
A. T. Hu	1965-70
B. H. Justice	1964
G. C. Karris	1965-68
S. Levine	1960-61
R. A. McDonald	1971-85
F. L. Oetting	1961
R. S. Orehotsky	1963-64
R. V. Petrella	1961-62
E. W. Phillips	1963-66
J. A. Rizos	1962-63
G. C. Sinke	1962,65,69,70
A. C. Swanson	1962-64
A. N. Syverud	1963-84
H. K. Unger	1963-64
E. A. Valenzuela	1975-81
L. C. Walker	1971-73
D. U. Webb	1967-68
S. K. Wollert	1963-65

We also wish to mention the valuable assistance in the typing of these Tables of Norma Dumont, 1959-64; Viola E. Harrington, 1964-66; Carol S. Scheffier, 1966-67; Wildene B. Harris, 1967-68; Mary J. Walter, 1968-71; and for the time period of 1971-78 of Joan Weldon, Cheri Snow, Barbara Boman, Sheila Knoerr, Patricia Grochowski, and Lisa Ittner. For the years 1978–1985 Betty Clark, Jan Crouch, and Rhoda Toth have typed the tables. Isabel Carr provided valuable services to the group in abstracting, searching and ordering documents, and proofreading the Tables for the Second Edition. For the period 1978–1985 Dana Donley, Debbie Simpson, Marge Sheets, Barbara Meier, Diana Scribner, and Anne Schmidt have provided similar assistance. Milton D. Marks was very instrumental in all computer aspects of this project in the 1980's.

In the time period of 1985 to 1998, technical contributions have been made by Stanley Abramowitz and David Neumann. Additional help in literature searching, data collection, and data entry has been provided by Cindy Jackson, Rhoda Levin, and Sabina Crisen.

3. Notation and Terminology

The symbols and terminology for physicochemical quantities and units are those recommended by IUPAC through its Physical Chemistry Division.[9,10] For the thermodynamic notation needed but not specified by these two sources, the recom-

mendations of the Bulletin of Chemical Thermodynamics[11] are used. Similarly, for spectroscopic nomenclature, the common practice of Moore[12] and Herzberg[13-16] is followed.

3.1. Definition of the Standard State

This description of the standard state is an abbreviated version of that given by the IUPAC Physical Chemistry Division.[10]

Absolute values of some thermodynamic quantities are unknown. Only changes in values caused by changes in parameters such as temperature and pressure can be determined. It is therefore important to define a base line for substances, to which the effect of such variations may be referred. The standard state is such a base line. The properties of these standard states are indicated by use of the symbol°. For a pure substance the concept of standard state applies to the substance in a well-defined state of aggregation at a well-defined but arbitrarily chosen standard pressure.

Historically, the defined pressure for the standard state, i.e., the standard-state pressure, had been one standard atmosphere (101 325 Pa). With the growing use of SI units, continued use of the atmosphere is inconvenient. IUPAC has recommended that the thermodynamic data should be reported for a defined standard-state pressure of 100 000 Pa. The standard-state pressure in general is symbolized as $p°$. Previously all JANAF thermochemical publications prior to the Third Edition, $p°$ was taken as 1 atm. Beginning with the Third Edition of the JANAF Thermochemical Tables, $p°$ is taken as 100 000 Pa (1 bar). It should be understood that the present change in the standard-state pressure carries no implication for "standard pressures" used in other contexts, e.g., the convention that "normal boiling points" refer to a pressure of 101 325 Pa (1 atm).

The change of the customary value of $p°$ from 1 atm (101 325 Pa) to 1 bar (100 000 Pa) results in small alterations in standard values of some thermodynamic quantities for all substances. For condensed phases the magnitude of these alterations is nearly always negligible in comparison with the uncertainty of current data. However, the alterations in values of entropy and the Gibbs energy function for a pure gaseous substance and of the Gibbs energy of reaction for a reaction involving gaseous species may not be negligible. This will be discussed in detail later (Sec. 4.3).

Hence, in all the tables appearing in this publication the standard state for a pure gaseous substance is that of the substance as an (hypothetical) ideal gas at 1 bar; the standard state for a pure liquid substance is that of the pure liquid under a pressure of 1 bar; the standard state for a pure solid substance is that of the pure crystalline substance under a pressure of 1 bar.

Since an enthalpy measurement is made as a difference between an initial and a final state, the reference temperature for enthalpy must be arbitrarily chosen. It is taken to be 298.15 K in all tables. Refer to the discussion of types of thermochemical tables for further details (Secs. 4.2 and 6).

3.2. Symbols

States of aggregation

The symbols and their corresponding descriptions for the states of aggregation are exactly those given by IUPAC.[9,10] They are rewritten here for the convenience of the reader.

Single letters are used to denote the three basic states of aggregation, gas, liquid, and solid, while combinations of letters are used for more subtle descriptions of states.

g	gas or a vapor
l	liquid
s	solid
cd	condensed phase (i.e., either the solid or the liquid state)
fl	fluid (i.e., either the gaseous or the liquid state)
cr	crystalline solid; where polymorphism occurs, it may be necessary to augment the symbol cr with a descriptor for the crystal modification under discussion; the preferred descriptors are Roman numerals, with textual definition of the crystallographic significance of the numerals used
am	amorphous solid
vit	vitreous substance (a glass)
mon	monomeric form
pol	polymeric form (in many cases the monomeric or polymeric character of the entity will be clear from the context without the symbol and the symbol should be used only in cases where ambiguity might result)
sln	solution; in many contexts it will be clear whether a liquid solution or a solid solution is meant, but where this is unclear it must be made clear by supplemental notation
aq	solution in which water is the solvent (an aqueous solution); in the past this symbol has sometimes been used to denote an infinitely dilute aqueous solution, but infinite dilution should henceforward be denoted by the extra symbol ∞.
sat	saturated; the state of equilibrium between phases, whether of a pure substance or a system of more than one component.

Processes

The symbols and their corresponding descriptions for processes are exactly those given by IUPAC.[9,10] The remaining six processes are denoted by the symbols recommended by the Bulletin of Chemical Thermodynamics.[11] The use of special symbols to denote a process are as follows:

vap	vaporization (evaporation) of a liquid
sub	sublimation (evaporation) of a solid
fus	melting (fusion) of a solid
trs	transition of one solid phase to another
mix	the mixing of fluids
sol	the process of solution (dissolution)
r	chemical reaction in general

c	combustion reaction; also can denote critical properties
f	a reaction in which a compound is formed from its elements (formation)
at	a process in which a substance is separated into its constituent gaseous atoms (atomization)
dcm	a process in which a substance decomposes (not given by IUPAC)
dso	a process in which a substance dissociates (not given by IUPAC)
dim	a process in which a substance dimerizes (not given by IUPAC)
dil	the dilution of a solution
gt	glass transition (not given by IUPAC)
hyd	hydrolysis (not given by IUPAC)
ion	ionization (not given by IUPAC)

Fundamental Constants

c	speed of light in vacuum
h	Planck constant
N_A	Avogadro constant
e	elementary charge
F	Faraday constant
R	gas constant
T_0	absolute temperature of "ice point"
k	Boltzmann constant
c_2	second radiation constant

Units

cal	calorie
eV	electron volt
g-atom	a mole of atoms
J	joule
K	kelvin
kcal	kilocalorie
kJ	kilojoule
mol	mole
L	liter

Mathematical Quantities

ln logarithm to the base e
lg logarithm to the base 10 (log)

Spectroscopic Quantities

The spectroscopic symbols, use, and description follow the well-established practices of Moore[12] and Herzberg.[13–16] These sources provide more extensive discussion as to the meaning and use of the various spectroscopic quantities.

The measured quantities often are reported in the literature for a specific isotopic molecule. The thermochemical tables in this publication normally use spectroscopic information for a natural isotopic abundance "molecule." Care should be exercised in noting to which molecule the spectroscopic data pertains.

Å	Angstrom
AP	appearance potential
B_0, B_e	rotational constant
D	centrifugal distortion constant
D_0°	dissociation energy is defined as the enthalpy of the ground-state products relative to the lowest existing level of the molecule; $D_0^\circ = \Delta_{at}H^\circ$ (0 K).
E_i	ionization energy (IP)
E_{ea}	electron affinity (EA)
g_i	quantum (or statistical) weight of the ith electronic state; quantity is the product of the spin multiplicity and state degeneracy of the electronic level under consideration
I_A, I_B, I_C	principal moments of inertia of a molecule
k	Hooke's law force constant
n	number of potential maxima in an internal rotation; also refers to principal quantum number in describing energy levels of atoms
N	number of atoms in molecule
r_e	internuclear distance (for the "equilibrium" structure of the molecule)
V_0	potential barrier to internal rotation
α_e	first-order rotation-vibration interaction constant
ϵ_i	ith electronic energy level
σ	symmetry number
μ	reduced mass of the molecule
ν	observed vibrational fundamental
ω_e	vibrational fundamental for infinitesimal amplitude
$\omega_e x_e$, $\omega_e y_e$	vibrational anharmonicity constants

Thermodynamic and Other Quantities

A_r	relative atomic mass (atomic weight)
C_p	molar heat capacity at constant pressure
C_s	molar heat capacity at saturation
ΔU	change in internal energy
ΔG	change in Gibbs energy, $G = H - TS = U + PV - TS$
ΔH	change in enthalpy, $H = U + PV$
K	equilibrium constant
M_r	relative molecular mass (molecular weight)
p	pressure
T	temperature, in kelvin
t	temperature, in degrees Celsius (°C)
V	volume
Δ	indicates the increment in a given property for a given process or reaction, taken as the value for the final state (or sum for the products) less that for the initial state (or sum for reactants).
$\Delta_f H^\circ$	represents the standard enthalpy of formation, which is the increment in enthalpy associated with the reaction of forming the given compound from its elements in their reference states, with each substance in its thermodynamic standard state at the given temperature.

Experimental Method Techniques

dsc	differential scanning calorimetry
dta	differential thermal analysis
emf	electromotive force
esr	electron spin resonance
glc	gas-liquid chromatography
gpc	gel permeation chromatography
ir	infrared spectroscopy
nmr	nuclear magnetic resonance
tga	thermogravimetric analysis
LLE	liquid-liquid equilibria
VLE	vapor-liquid equilibria
VP/xxxx	vapor pressure/experimental technique
/ebul	= ebulliometric
/Knud	= Knudsen effusion
/stat	= static
/Kems	= Knudsen effusion-mass spectrometry
/Kete	= Knudsen effusion-torsion effusion
/tran	= transpiration
/Lang	= Langmuir free evaporation
/Lams	= Langmuir-mass spectrometry

3.3. Relative Atomic Masses and Natural Isotopic Composition of the Elements

The Table of Atomic Weights of the Elements 1981[7a] is reprinted below. Added to this list are the relative atomic masses for the electron (e-) and deuterium (D). The relative atomic mass for the electron is given by Cohen and Taylor.[8a]

The 1981 report on atomic weights[17] includes a complete review of the natural isotopic composition of the elements and also tabulates the relative atomic masses for selected radioisotopes. This information is required for the conversion of spectroscopic data from that corresponding to specific isotopes to the naturally occurring isotopic abundance. For tabulations issued with dates later than 1985, more recent values are used.

As in the IUPAC report, values in parentheses are used for radioactive elements whose relative masses cannot be quoted exactly without knowledge of the origin of the elements; the value given is the atomic mass number of the isotope of that element of longest known half life. Alternatively, the relative atomic mass of the isotope with the longest known half life or that of a commonly used isotope could be listed, since the relative atomic masses of the individual isotopes are accurately known.

As mentioned in the Introduction (Sec. 1), for tables issued since the Third Edition, values of the molecular masses are based on the 1993 IUPAC recommendations.

NIST-JANAF THERMOCHEMICAL TABLES

Table of relative atomic masses of the elements, 1981
[Pure Appl. Chem. 55, 1101 (1983), alphabetical order, based on the relative atomic mass, $A_r(^{12}C) = 12$]

Name	Symbol	atomic number	Relative atomic mass
Actinium	Ac	89	227.0278
Aluminum	Al	13	26.98154
Americium	Am	95	(243)
Antimony (Stibium)	Sb	51	121.75
Argon	Ar	18	39.948
Arsenic	As	33	74.9216
Astatine	At	85	(210)
Barium	Ba	56	137.33
Berkelium	Bk	97	(247)
Beryllium	Be	4	9.01218
Bismuth	Bi	83	208.9804
Boron	B	5	10.81
Bromine	Br	35	3579.904
Cadmium	Cd	48	112.418
Caesium	Cs	55	132.9054
Calcium	Ca	20	40.08
Californium	Cf	98	(251)
Carbon	C		12.011
Cerium	Ce	58	140.12
Chlorine	Cl	17	35.453
Chromium	Cr	24	51.996
Cobalt	Co	27	58.9312
Copper	Cu	29	63.546
Curium	Cm	96	(247)
Deuterium	D	1	2.014102
Dysprosium	Dy	66	162.50
Einsteinium	Es	99	(252)
Electron	e-		0.000 548 58
Erbium	Er	68	167.26
Europium	Eu	63	151.96
Fermium	Fm	100	(257)
Fluorine	F	9	18.998403
Francium	Fr	87	(223)
Gadolinium	Gd	64	157.25
Gallium	Ga	31	69.72
Germanium	Ge	32	72.59
Gold	Au	79	196.9665
Hafnium	Hf	72	178.49
Helium	He	2	4.00260
Holmium	Ho	67	164.9304
Hydrogen	H	1	1.00794
Indium	In	49	114.82
Iodine	I	53	126.9045
Iridium	Ir	77	192.22
Iron	Fe	26	55.847
Krypton	Kr	36	83.80
Lanthanum	La	57	138.9055
Lawrencium	Lr	103	(260)
Lead	Pb	82	207.2
Lithium	Li	3	6.941
Lutetium	Lu	71	174.967
Magnesium	Mg	12	24.305
Manganese	Mn	25	54.9380
Medelevium	Md	101	(258)
Mercury	Hg	80	200.59
Molybdenum	Mo	42	95.94
Neodymium	Nd	60	144.24
Neon	Ne	10	20.179
Neptunium	Np	93	237.0482
Nickel	Ni	28	58.69
Niobium	Nb	41	92.9064
Nitrogen	N	7	14.0067
Nobelium	No	102	(259)
Osmium	Os	76	190.2
Oxygen	O	8	15.9994
Palladium	Pd	46	106.42
Phosphorus	P	15	30.97376
Platinum	Pt	78	195.0
Plutonium	Pu	94	(244)
Polonium	Po	84	(209)
Potassium (Kalium)	K	19	39.0983
Praseodymium	Pr	59	140.9077
Promethium	Pm	61	(145)
Protactinium	Pa	91	231.0359
Radium	Ra	88	226.0254
Radon	Rn	86	(222)
Rhenium	Re	75	186.207
Rhodium	Rh	45	102.9055
Rubidium	Rb	37	85.4678
Ruthenium	Ru	44	101.07
Samarium	Sm	62	150.36
Scandium	Sc	21	44.9559
Selenium	Se	34	78.96
Silicon	Si	14	28.0855
Silver	Ag	47	107.8682
Sodium (Natrium)	Na	11	22.98977
Strontium	Sr	38	87.62
Sulfur	S	16	32.06
Tantalum	Ta	73	180.9479
Technetium	Tc	43	(98)
Tellurium	Te	52	127.60
Terbium	Th	65	158.9254
Thallium	Ti	81	204.383
Thorium	Th	90	232.0381
Thulium	Tm	69	168.9342
Tin	Sn	50	118.69
Titanium	Ti	22	47.88
Tungsten (Wolfram)	W	74	183.85
(Unnilhexium)	(Unh)	106	(263)
(Unnilpentium)	(Unp)	105	(262)
(Unnilquadium)	(Unq)	104	(261)
Uranium	U	92	238.0289
Vanadium	V	23	50.9415
Xenon	Xe	54	131.29
Ytterbium	Yb	70	173.04
Yttrium	Y	39	88.9059
Zinc	Zn	30	65.38
Zirconium	Zr	40	91.22

3.4 Fundamental Constants and Conversion Factors

The numerical values of the fundamental constants used in our calculations are those obtained by Cohen and Taylor[8a] based on a least-squares adjustment of data existing in 1973. These values have been adopted by CODATA.[8a]

As mentioned in the Introduction (Sec.1), for tables issued since the Third Edition, values of the fundamental constants are based on the 1986 CODATA recommendations.[8b]

Fundamental constants

Quantity	Symbol	Value[a]
Speed of light in vacuum	c	299 792 458(1.2) m s^{-1}
Planck constant	h	6.626 176(36) × 10^{-34} J s
	$h/2\pi$	1.054 588 7(57) × 10^{-34} J s
Avogadro constant	N_A	6.022 045(31) × 10^{23} mol^{-1}
Elementary charge	e	1.602 189 2(46) × 10^{-19} C
Faraday constant, $N_A e$	F	9.648 456(27) × 10^4 C mol^{-1}
Absolute temperature of "ice point," O °C	T_O	273.150 0 K
Molar gas constant	R	8.314 41(26) J mol-1 K^{-1}
Boltzmann constant, RN_A^{-1}	k	1.380 662(44) × 10^{-23} J K^{-1}
Second radiation constant, hck^{-1}	c_2	1.438 786(45) × 10^{-2} m K

[a]Numbers in parentheses are the one standard deviation uncertainties in the last digits of the quoted value.

Conversion factors for energy-related units. 1973 CODATA constants

	kJ mol^{-1}	kcal mol^{-1}	eV (per molecule)	cm^{-1}	MHz
1 kJ mol^{-1}	1	0.239 005 7	0.010 364 35	83.593 47	2.506 069 × 10^6
1 kcal mol^{-1}	4.184	1	0.043 364 45	349.755 1	1.048 539 × 10^7
1 eV (per molecule)	96.4846	23.06036	1	8065.479	2.417 970 × 10^8
1 MHz	3.990 313 × 10^{-1}	9.537 077 × 10^{-8}	4.135 701 × 10^{-9}	3.335 641 × 10^{-5}	1
1 cm^{-1}	0.011 962 66	2.859 144 × 10^{-7}	1.239 852 × 10^{-4}	1	2.997 924 × 10^4
1 K (degree)	8.314 41 × 10^{-3}	1.987 19 × 10^{-7}	8.617 349 × 10^{-5}	0.695 030 4[a]	2.083 649 × 10^4
1 hartree	2625.500	627.509 5	27.211 606	2.194 746 × 10^5	6.579 684 × 10^9
1 rydberg	1312.750	313.754 7	13.605 803	1.097 373 × 10^5	3.289 842 × 10^9

[a]This value is inverse of the second radiation constant c_2; $(hc/k)^{-1} = c_2^{-1} = 0.695\ 030\ 4$.

3.5. Temperature Scale

Since the NIST-JANAF Thermochemical Tables deal with properties that vary with temperature, the temperature scale is of significance. The International Temperature Scales are devised to approximate, as closely as possible, the absolute thermodynamic (kelvin) temperature suggested by W. Thomson (Lord Kelvin) in 1854. The International Temperature Scale is established by the Comité International des Poids et Mesures (International Committee of Weights and Measures).

There have been four international temperature scales: The International Temperature Scale of 1927,[18] The International Temperature Scale of 1948 which was renamed the International Practical Temperature Scale of 1948 (IPTS-48) in 1960,[19–20] The International Practical Temperature Scale of 1968 (IPTS-68)[21] and The International Temperature Scale of 1990 (ITS-90).[22]

Our concern in the preparation of the NIST-JANAF Thermochemical Tables is to adjust any experimental measurements to the thermodynamic scale. In practice, this means converting to the ITS-90 scale since it is the currently accepted closest approximation to the thermodynamic scale.

To facilitate temperature adjustments, the article by Corruccini[19] was used for the 1927 to 1948 conversions and the article by Douglas[23] for the 1948 to 1968 conversion. Guildner and Edsinger[24] included a plot showing the deviation of IPTS-69 from the thermodynamic temperatures from 273.16 to 730 K. For conversions to the current scale (ITS-90), there are numerous articles which discuss the conversion of experimental data or smoothed results to the new temperature scale.

Ideal-gas tables of thermodynamic properties derived from statistical mechanics are based on the thermodynamic temperatures (as well as on the values of the physical constants used) and are hence independent of any practical temperature scale. The enthalpy of formation, Gibbs energy of formation, and logarithm of the equilibrium constant might depend on temperature-adjusted data.

For condensed phase tables, the temperature scale conversion is often not necessary and is not made since the correction would be small compared with the uncertainty in the data.

4. Reference States and Conversions

There are three types of tables included in this publication: single-phase, multiphase, and reference state tables. The tables are clearly labeled as to the type at the top of each page and by the state designations associated with the chemical formula. The reference state can involve a single phase or multiphases. The major difference between a multiphase table and a single-phase table is the existence of a discontinuity in each function (or in its first derivative) at a first-order transition temperature.

4.1. Reference State

A related set of thermodynamic property tables requires that there be a reference table of the thermodynamic properties for each element to which all other forms of that element or any compound involving that element may be referred. If the temperature range of interest (0 K to 6000 K herein) can be represented by a single phase for that material (say hydrogen) the tabulated values in the reference table will be smooth and regular. If the temperature range of interest includes more than one phase (say magnesium), there will be a solid phase (from 0 K to 923 K, the melting temperature), a liquid phase (923 K to 1378 K, where the vapor pressure reaches 1 bar), and a gas phase (1378 K to 6000 K), and the tabulated values in the reference table will be discontinuous at these temperatures or phase boundaries. Practical usage dictates that in so far as possible the phase most stable at 1 bar pressure be selected. This practice is followed in these tables, and does lead to discontinuities in the thermodynamic functions. Attention is called to these discontinuities in the reference state tables by insertion of a comment as to the type of transition at the temperature of the phase transition.

Since these tables deal with ideal gases, the pressure is really the fugacity. Calculating a boiling temperature as the temperature at which $\Delta_{vap}G^\circ = 0$ for the process Mg(l)→Mg(g) corresponds to an (ideal) fugacity of 1 bar. This will differ from the real (observed) boiling point at 1 bar which is also different from the real (observed) boiling point at 1 atm. Each of these "three boiling points" corresponds to a different $\Delta_{vap}G^\circ$ value.

With the use of f and °, as in Δ_fH°, the implication is that both the compound in question and its constituent elements are in standard states and that the elements, moreover, are in their reference states; for any given temperature the reference states of the elements will normally be those that are stable at the chosen standard-state pressure and at that temperature. A resulting feature of tabulations of Δ_fH° and Δ_fG° as functions of temperature for compounds is that discontinuous changes are sometimes to be seen; these correspond to changes in the stable reference states of the elements, as phase-transition temperatures are passed. Thus, values of Δ_fH° (SO_2Cl_2,g) would show discontinuous changes at three temperatures corresponding to the transitions S(cr,I)→S(cr,II), S(cr,II)→S(l), and S(l)→1/2 S_2(g), where I refers to rhombic and II to monoclinic crystal forms.

4.2. Single-Phase and Multiphase Tables

A multiphase table contains the data for two or more phases of a pure substance. Each phase is limited to the temperature range in which it is more stable (i.e., has a lower Δ_fG° than the other phases in the table). There are discontinuities in the properties C_p°, S°, and H° at the temperatures where each phase transforms ($\Delta G^\circ = 0$) to the next phase. Alternatively, the properties of a pure substance can be given in a series of tables where each table is devoted to a single phase. Single-phase tables do not have discontinuities in the properties C_p°, S°, and H° at transition temperatures. Moreover, the properties are extrapolated beyond the transition temperatures into regions where that phase is less stable than its other phases. These characteristics of continuity and extrapolation of properties lead directly to the advantages and problems of single-phase tables. The enthalpy of formation and Gibbs energy of formation may have discontinuities, even in single-phase tables, corresponding to transitions in the reference states.

Single-phase tables are more convenient than multiphase tables in certain computer applications. Interpolation and approximation (curve fitting) apply directly to the continuous properties in a single-phase table. Multiphase tables must first be divided into segments using the stored values of the transition temperatures; then interpolation and approximation must be limited to the temperatures in the pertinent segment.

Single-phase tables are essential in uses that involve unstable phases. This includes phases that persist in a metastable region or those that are unstable at all temperatures. [Such cases abound in the real world.] Single-phase tables are often applied to solid-solid or solid-liquid equilibrium in mixtures, where an unstable phase is "stabilized" in the presence of other components. Analysis of such equilibria often requires liquid or solid properties that are many hundreds of degrees into the metastable region of each pure phase. Single-phase tables are designed to supply these properties, but their preparation is not trivial.

The NIST-JANAF Thermochemical Tables often include estimated glass transitions in the liquid tables. The glass temperature is usually assumed to be ~0.7 times the melting temperature. The heat capacity of the glass is usually assumed to be equal to that of the stable crystalline phase, since existing glass data show a decrease in C_p° to values near those of the crystal. Such tables are, in fact, not single-phase tables but two-phase glass-liquid tables.

The glass transition is of practical concern when thermochemical tables are used near the glass transition temperature of any of the pure liquids. Although the ratio of the glass temperature to the melting temperature can vary from perhaps 0.35 to >0.8, it often is ~0.7. Temperatures this low are not uncommon when tables for liquids are used in the analysis of binary or multicomponent phase diagrams.

It is important to ask whether glass transitions should be included in liquid tables intended for such use. Estimated glass transitions are included for two reasons: the transition is usually observed in supercooled liquids and its inclusion avoids an entropy paradox. The first reason presumes that

glass transitions do occur but cannot be observed in liquids that readily crystallize. The more compelling reason is the avoidance of the paradox in which the entropy of the supercooled liquid (a disordered state) becomes less than that of the stable crystalline state.

The choice remains as to what temperature and what phase should be used as the reference point for enthalpy in the extrapolated single-phase tables. Since 298.15 K was adopted as the reference temperature for multiphase and reference state tables, there is strong incentive for retention of that temperature in single-phase tables. The choice has been made to have the reference at the same arbitrary point in each phase. Thus, the JANAF Thermochemical Tables use a reference temperature of 298.15 K in the table for the high-temperature phase even when that phase is not stable at 298.15 K.

Enthalpies at all temperatures depend on the arbitrary extrapolations needed to relate the observed data to the reference temperature. Each single-phase table has a different reference $\Delta_f H°$ dependent on an arbitrary extrapolation of enthalpy.

For the reference temperature of 298.15 K, the enthalpy at $T \rightarrow 0$ is always negative. This means that the function $-(G° - H)/T$ approaches positive ∞ at $T \rightarrow 0$ and is therefore difficult to interpolate near $T \rightarrow 0$.

4.3. Conversion to SI Units and the Standard-State Pressure

In all previous JANAF Thermochemical Tables, the standard-state pressure was one atmosphere (101 325 Pa) and the unit of energy was the thermochemical calorie (4.184 J). For this publication, the standard-state pressure is changed to one bar (100 000 Pa) and the energy unit to the joule. The values from previous JANAF tabulations have been converted as described below. This information is provided not only to make clear the correspondence between this publication and previous JANAF Thermochemical Tables but also to assist the reader in making comparisons with other tables. This information is the same as that provided in "The NBS Tables of Chemical Thermodynamic Properties."[6]

Conversion of Values in Calories to Joules

For the energy units the defined conversion factor of 4.184 $J \cdot cal^{-1}$ is used.

Conversion for Change in Pressure

The following expressions define the effect of pressure on the properties of all substances.

$$(\partial H/\partial p)_T = V - T(\partial V/\partial T)_p = V(1 - \alpha T),$$
$$(\partial C_p/\partial p)_T = -T(\partial^2 V/\partial T^2),$$
$$(\partial S/\partial p)_T = -V\alpha = -(\partial V/\partial T)_p,$$
$$(\partial G/\partial p)_T = V,$$
$$\alpha \equiv (1/V)(\partial V/\partial T)_p$$

For the small pressure change from 1 atm to 1 bar, the pressure coefficients may be taken as constants for condensed phases. There are no condensed phase cases in this publication for which the pressure coefficients are large enough to affect the tabulated values. Typical values of α for solids are 10^{-5} to 2×10^{-4} K^{-1} and $V < 10^{-3}$ m^3 mol^{-1}. For ideal gases, $V = RT/p$ and $\alpha = R/pV = 1/T$. The pressure coefficients for gases are large enough to affect high-accuracy data. In practice the only properties tabulated here that are affected are $S°(T)$ and $-(G°(T) - H°[298.15\ K])/T$ for all gases, and $\Delta_f G°(T)$ and lg K_f for any substance whenever gases are involved.

The conversion equations used for the change in standard-state pressure are listed below together with some that apply to thermal functions. Superscripts ° and * denote values at 1 bar and 1 atm, respectively. These equations apply to the small change in pressure from 1 atm to 1 bar.

For all substances, exactly for ideal gases and within the limit of experimental inaccuracy for all other phases:

$$\Delta_f H°(T) - \Delta_f H*(T) = 0,$$
$$[H°(T) - H°(T_1)] = [H*(T) - H*(T_1)] = 0,$$
$$C_p°(T) - C_p*(T) = 0,$$

where T_1 is a reference temperature.

For condensed phases, within the limit of experimental inaccuracy:

$$S°(T) - S*(T) = 0$$
$$G°(T) - G*(T) = 0$$

For substances that are gaseous:

$$S°(T) - S*(T) = R \ln p*/p°$$
$$= R \ln \frac{101325}{100\,000} = 0.109\ 444\ J \cdot K^{-1}\ mol^{-1}.$$

For substances that are gaseous at T but may or may not be gaseous at T_1:

$$-[G°(T) - H°(T_1)]/T + [G*(T) - H*(T_1)]/T = R \ln p*/p° \text{ as for } S.$$

$$[G°(T) - G°(T_1)] - [G*(T) - G*(T_1)] = R\,(T - T_j) \ln p*/p°,$$

where $T > T_j \geq T_1$ and T_j is the temperature at which the function begins to apply to the ideal gas, usually the boiling temperature at 1 bar.

For each substance with gases in its formation reaction:

$$\Delta_f G°(T) - \Delta_f G*(T) = -\delta RT \ln 1.013\ 25 = -0.032\ 63\ \delta\ kJ\ mol^{-1} \text{ at } 298.15\ K.$$

where δ is the net increase in the number of moles of gas in the formation reaction.

Conversions for Entropies of Gases

To convert from:	$S°$(g,0.1 MPa) / J·K^{-1} mol^{-1}	$S*$(g,1 atm) / cal·K^{-1} mol^{-1}	$S^\dagger$ (g,1 atm) / J·K^{-1} mol^{-1}
To:	Use		
$S°$(g,0.1 MPa) / J·K^{-1} mol^{-1}	= $S°$	4.184($S*$ + 0.026 157)	$S^\dagger$ + 0.109 442
$S^\dagger$ (g,1 atm) / J·K^{-1} mol^{-1}	= $S°$ - 0.109 442	4.184 $S*$	$S^\dagger$
S(g,0.1 MPa) / cal·K^{-1} mol^{-1}	= $S°$/4.184	$S*$ + 0.026 157	($S^\dagger$ + 0.109 442)/4.184
$S*$(g,1 atm) / cal·K^{-1} mol^{-1}	= ($S°$ - 0.109 442)/4.184	$S*$	$S^\dagger$ /4.184

$S°$ entropy for a gas at 0.1 MPa in J·K^{-1} mol^{-1}.
$S*$ entropy for a gas at 1 atm in cal·K^{-1} mol^{-1}.
$S^\dagger$ entropy for a gas at 1 atm in J·K^{-1} mol^{-1}.

4.4. Boiling Temperature and the Standard-State Pressure

In these tables, the defined pressure for the standard state is 1 bar (100 000 Pa). As stated by IUPAC,[9] the present recommended change in the standard-state pressure carries no implication for "standard pressures" used in other contexts, e.g., the convention that "normal boiling points" refer to a pressure of 1 atm (101 325 Pa). Instances may occur where it is desirable to adopt yet other values for $p°$ and so all authors must clearly state the value adopted.

In these tables, the temperature at which $\Delta_r G° = 0$ for the process liquid to gas, refers to a fugacity of 1 bar. Typically the real (i.e., observed) boiling point (corresponding to a nonideal gas) is slightly higher. In many cases the experimental uncertainties in measuring a boiling point (at 1 bar) and the uncertainties in the calculated value due to uncertainties in the thermal functions make this difference meaningless. Such a situation exists whether the standard-state pressure is 1 bar or 1 atm.

The phrase "boiling point" must be used carefully for other reasons. Care must be exercised such that the boiling process is indeed defined. Two examples which illustrate this point are MgO and LiF. Magnesium oxide does not vaporize congruently (so that the total vapor pressure depends on the ambient oxygen potential), whereas LiF vaporizes congruently but monomer, dimer, and trimer species exist in the vapor.

5. Evaluation of Thermodynamic Data

Interconsistency

The basic aim of these thermodynamic property tables is to provide a related and consistent set of enthalpies of formation and Gibbs energies of formation. This allows the prediction of the enthalpy and Gibbs energy changes and the equilibrium constants for any reaction among the constituents of the tables.

The enthalpy of formation and Gibbs energy of formation are related to each other through the entropy of formation of the substance. Self-consistency can be assured by use of this constraint to derive any one property from selected values of the other two. The entropy, which is an absolute quantity in thermochemical calculations, is suitable for one of the selected properties. The enthalpy of formation is convenient for the other, since enthalpy of reaction is the most commonly measured link between different substances.

Enthalpy changes are relative quantities, so it is important to relate each substance to a consistent base. This is done by referring each enthalpy of formation to the chemical elements in their standard reference states. By convention, the enthalpy of formation of an element in its standard reference state is zero at all temperatures.

The reference state table may involve a single phase or several phases and examples of both kinds are found in this compilation. For elements which are solid at room temperature, the reference state is normally the stable solid state(s) up to the melting point, the liquid up to the boiling point at 1 bar, and thereafter the gas phase which may be monatomic or diatomic. For other elements, the choices for the reference states are:

(1) the ideal monatomic gas for the inert rare gases and the electron gas He, Ne, Ar, Kr, Xe, Rn, and e^-. The classical statistical mechanical values are assumed for $H°(T) - H°(0)$ for the electron.

(2) the ideal diatomic gas for the following gases: H_2, D_2, N_2, O_2, F_2, and Cl_2.

(3) crystalline white phosphorus and the ideal diatomic gas, $\frac{1}{2}P_2$(g). The early JANAF publications used red phosphorus as the reference state. Although red phosphorus is the more stable form, it is less well characterized and its properties are less reproducible.

(4) the ideal diatomic gas combined with the appropriate condensed phases for Br_2, I_2, and S; for sulfur, the gaseous portion of the reference state is $\frac{1}{2}S_2(g)$.

(5) graphite (Acheson-spectroscopic grade) for carbon at all temperatures.

These choices are arbitrary and vary in different compilations. Enthalpies or Gibbs energies of formation taken from different sources should be converted to common reference states before use.

The establishment of reference states is the first step in any scheme for interconsistency. The next step, ideally, would be to solve simultaneously for all $\Delta_f H°$, $\Delta_f G°$, $S°$ using all the suitable data for $\Delta_r H°$, $\Delta_r G°$, $\Delta_r S°$, and $S°$. This would provide values for enthalpies, Gibbs energies, and entropies which, when combined, would yield the minimum overall deviations from the measured values. Simultaneous solution is limited in practice to small groups of interrelated substances.

We have used this simultaneous approach in a limited way for treating groups of interrelated fluorides. Dr. John L. Haas, Jr. (U.S. Geological Survey) has treated, simultaneously, the data for some geologically important systems as a function of temperature and pressure.[25] Dr. J. Brian Pedley (University of Sussex) has treated $\Delta_f H°$ data for several systems, the most pertinent involving all the diatomic oxides.[26] Dr. Vivian Parker and Dr. David Garvin (NBS) have refined the latter method and applied it to some species that were adopted by CODATA.[27] JANAF policy is to use the results of these treatments.

Since simultaneous solution has not been attempted for all substances it is necessary to fix, simultaneously when possible, certain key values for common substances. These are then used in the usual sequential way to help fix other substances. JANAF policy is to adopt the key values recommended by the CODATA Task Group for Key Values in Chemical Thermodynamics.[28] Exceptions to this policy only occur when additional recent data are available.

Because of the many revisions of these tables, perfect interconsistency is not always attained. However, any inconsistency of the tables is a prime concern and is a cause for revision if the effects are of the same order of magnitude as the stated uncertainties.

An approximate type of consistency relates to trends in properties within families in the periodic table. Expected trends can aid both in estimation of missing data and in evaluation of observed data, for example, in a series from fluoride to iodide or from polyhalide to monohalide.

5.1. General Evaluation Techniques

Heat Capacities and Enthalpy Difference

The evaluation of reported values is a judgmental process, but the analysis should be as objective as possible and therefore certain ground rules must be established. The first step involves the examination of a plot of all information so that a general idea of the agreement can be visually obtained. If certain data sets differ from the majority, they are examined for possible causes of the difference. Calibration data, sample purity, and experimental scatter are checked. If the source of error can be located, the data are given appropriately less weight. Otherwise all data of equal reliability are considered equal, even if they disagree. Such data are then smoothed by a weighted least-squares curve fit. Enthalpy data are smoothed similarly and heat capacities are derived exactly from the differentiated polynomial. The smoothing of enthalpy data often requires constraining the fit so that it passes through zero at the reference temperature. Additional constraints are often used to fix the heat capacity at 298.15 K or to join enthalpy data smoothly with low-temperature heat capacities.

Transitions

The evaluation of solid-state transitions involves first the recognition of the type of transition, which may not always be obvious. A first-order transition such as fusion involves a discontinuous change of enthalpy and entropy at the transition point, whereas second-order transitions involve only discontinuities in heat capacity. Because of impurities and other factors, first-order transitions often do not occur sharply at one temperature; instead, they spread a little on either side and are sometimes difficult to distinguish from λ-type second-order transitions.

Many enthalpies of fusion and enthalpies of solid-state transitions are obtained from enthalpy measurements. Here the enthalpies are given directly by the difference in enthalpy at the transition temperature. Normally, the enthalpy above and below can be smoothly extended to the temperature of transition, although the transition temperature may not be clearly obtainable from the enthalpy data.

The enthalpies of the transitions involving vaporization and sublimation are evaluated from equilibrium data by the second- and third-law methods. When reliable calorimetric measurements are available, the adopted enthalpy of transition is usually based on them.

Equilibrium

Perhaps the most significant facts to be established in evaluating equilibrium data are whether equilibrium was attained and whether the process was properly described. For example, in a sublimation process the most accurate measurements are valueless if the vapor phase is not uniquely defined. If polymerization or breakdown might have occurred, it is important to establish the exact reaction first. Because mass spectroscopy has shown that vapor phases are often extremely complex, it is almost a requirement that the vapor composition be established by a mass spectrometer before equilibrium data can be accepted. Some methods of measurement are less accurate than others and should be given less weight. For example, equilibria determined in a mass spectrometer may have significant uncertainty because of the approximations involved in obtaining absolute pressures. On the other hand, measurements of the electromotive force of reversible cells can have great accuracy. Mass spectra provide identification

of the vapor species while a very precise emf measurement tells nothing as to the reaction which is occurring. Each method has inherent limitations; these may be more critical in some uses than in other uses. Clues to the existence of these limitations often appear in the second- and third-law analyses.

The Second-Law Method

Starting from the equation $\Delta G^\circ = -RT \ln K$, by differentiation with respect to T and substitution of $d(\Delta G^\circ)/dT = -\Delta S^\circ$, we obtain $\Delta H^\circ = RT^2 d(\ln K)/dT$, the well-known van't Hoff equation. By substituting $dT = -T^2 d(1/T)$, one obtains $\Delta H^\circ = -R\, d(\ln K)/d(1/T)$; thus, the slope of ln K versus $1/T$ plot is $-\Delta H^\circ/R$. If ΔH° is constant, then the slope is constant and the plot is a straight line. Since the variation of ΔH° with temperature is often quite small, it is customary to assume a straight-line relationship. This method of obtaining enthalpies of reaction from equilibrium measurements is known as a "second-law" calculation. For greatest accuracy the equilibrium measurements should extend over a wide range of temperature, and in this case ΔH° is usually not constant.

Curvature corrections can be applied by assuming a specific form for the variation of ΔH° with temperature. In this manner we can calculate $\Delta_f H^\circ$ (298.15 K) from $\Delta_f H^\circ$ (T). The effects of such corrections may be of significance. It should be noted that the second law cannot be applied to a single observation, but the third-law method, which is described below, can be so used. The second-law method also can be applied when only relative values of the equilibrium constant are available, for example, from mass-spectroscopic intensity measurements.

The Third-Law Method

The "third-law" method is based on a knowledge of the absolute entropy of the reactants and products. It allows the calculation of a reaction enthalpy from each data point when the change in the Gibbs energy function for the reaction is known. The Gibbs energy function used here is defined as

$$\text{gef}(T) = [G^\circ(T) - H^\circ(298.15\ \text{K})]/T$$

and is easily calculated from the relation

$$\begin{aligned} S^\circ/(T) &= -[G^\circ(T) - H^\circ(T)]/T \\ &= [H^\circ(T) - H^\circ(298.15\ \text{K})]/T \\ &\quad - [G^\circ(T) - H^\circ(298.15\ \text{K})]/T \end{aligned}$$

thus,

$$\text{gef}(T) = -S^\circ(T) + [H^\circ(T) - H^\circ(298.15\ \text{K})]/T$$

From the definition we can write for the change in a reaction

$$\Delta G^\circ/T = \text{gef}(T) + \Delta H^\circ(298.15\ \text{K})/T = -R \ln K,$$

thus,

$$\Delta H^\circ(298.15\ \text{K})/T = -R \ln K - \Delta\text{gef}(T),$$

where Δgef signifies gef(products) − gef(reactants).

In the NIST-JANAF Thermochemical Tables, Gibbs energy functions are based on an enthalpy reference temperature of 298.15 K and thus yield enthalpy changes at 298.15 K regardless of the temperature of the reaction. It should be noted that the Gibbs energy function in a single-phase table is based on the enthalpy of that phase at 298.15 K even though the phase may not be stable at 298.15 K. This differs from the usual convention of combining all condensed phases into one multiphase table such that the enthalpy of reaction refers to the phase stable at the reference temperature. In the JANAF tables the functions always refer to the designated phase for 298.15 K regardless of its stability. For example, if the vapor pressure over liquid copper is analyzed using Cu(l) Gibbs energy functions, the result is the enthalpy of vaporization of the liquid at 298.15 K. To calculate the enthalpy of sublimation of Cu(cr) it is necessary to add the enthalpy of fusion at 298.15 K, which is the difference in the enthalpy of formation of Cu(l) and Cu(cr) at 298.15 K. It should also be noted that Gibbs energy functions are always negative, thus the negative of the function is usually tabulated and the proper sign must be remembered when using these functions.

The analysis of data by the third-law method is generally considered superior to the second-law analysis. It is definitely superior if the Gibbs energy functions are accurately known because each equilibrium point yields one value for the enthalpy change. These values will often reveal trends that indicate nonequilibrium or erroneous values in the equilibrium constants of a set of data. If the data are good, the second-law value should agree. When the Gibbs energy functions are estimated, the third-law values derived from them must be handled carefully. Values that are constant and that agree with the second-law enthalpy indicate that the Gibbs energy functions and equilibrium data are mutually consistent. A drift with temperature of the third-law values indicates errors in either the data or the functions. The magnitude of such drifts is often given in the table write-up and represents the entropy change required to bring the second- and third-law values into agreement. If the drift is within the uncertainty of the experimental entropy, then the data are acceptable. Drifts that are much larger than reasonable entropy errors generally indicate failure to attain equilibrium or improperly estimated Gibbs energy functions.

We have found a combination of the two methods to be so valuable that a third-law calculation is always accompanied by a second-law treatment of the same data. The calculation is done in ascending temperature order to give $\Delta_f H^\circ$(298.15 K) and its deviation from the mean along with the calculated log K and its deviation from the least-square line. Third-law analysis enables bad points to be seen as deviations from the general trend of the differences; thus the method can be used even when the Gibbs energy functions are estimated. If these bad points are located on the ends of the data set, the second-law line often fits them quite well and by itself does not arouse suspicion. But the dropping of such points can bring widely discordant ΔH° values into agreement with each other and often with the third-law values.

In our analysis of equilibrium data, tabulations for both the second- and third-law results are normally given. In addition, we often list values for the drift of δS, as defined by

$$- \text{drift} = \delta S = \Delta_r S^\circ \text{ (2nd law, 298.15 K)} - \Delta_r S^\circ \text{ (3rd law, 298.15 K)}$$

δS previously called a drift (in $\Delta_f H^\circ$), gives a direct comparison of the deviation of the calculated second-law entropies from our adopted functions. The current policy is to use δS rather than drift. $\Delta_r S^\circ$ (2nd law, 298.15 K) is not calculated, however, via the usual second-law method or the method.[29,31] It is instead derived from the slope of the assumed linear temperature dependence of the deviations from the mean of the third-law enthalpies of reaction. Our experience indicates that this method agrees closely, but not exactly, with the method.

6. Construction of the Tables

The NIST-JANAF Thermochemical Tables consist of thermal functions and formation functions, both of which are temperature dependent. The thermal functions consist of heat capacity, enthalpy increments, entropy, and Gibbs energy function. The normal relationships hold between thermal functions:

$$H^\circ(T) = \int_0^T C_p^\circ(T)\mathrm{d}T,$$

$$S^\circ(T) = \int_0^T [C_p^\circ(T)/T]\mathrm{d}T,$$

$$[G^\circ(T) - H^\circ(298.15\text{ K})]/T = -S^\circ(T) + [H^\circ(T) - H^\circ(298.15\text{ K})]/T.$$

The formation functions consist of enthalpy of formation, Gibbs energy of formation, and the logarithm of the equilibrium constant of formation. Enthalpies of formation at temperatures other than 298.15 K require a knowledge of enthalpies of the reference elements:

$$\Delta_f H^\circ(T) = \Delta_f H^\circ(298.15\text{ K}) + [H^\circ(T) - H^\circ(298.15\text{ K})]_{\text{compound}} - \Sigma[H^\circ(T) - H^\circ(298.15\text{ K})]_{\text{elements}}.$$

The Gibbs energy of formation is readily calculated from the enthalpy of formation when the entropies of the elements are known. Thus

$$\Delta_f G^\circ(T) = \Delta_f H^\circ(T) - T\{S^\circ(T)_{\text{compound}} - \Sigma S^\circ(T)_{\text{elements}}\}.$$

The logarithm of the equilibrium constant of formation is then found from the relation $\Delta_f G^\circ(T) = -RT \ln K_f$.

Solid Phase Thermal Functions

The solid phase thermal functions are derived from recommended heat capacity and/or enthalpy increment values. Although the NIST-JANAF Thermochemical Tables place more emphasis on high temperatures ($T > 298.15$ K), it is desirable have data in the temperature range of $T \rightarrow 0$ to 298.15 K. There is no basic difference in evaluating low-temperature data, but many more heat capacity points are needed to describe fully the large curvature in the temperature dependence of the heat capacity. In order to evaluate the enthalpy increment it is necessary to start with the temperature $T = 0$ and integrate up to 298.15 K; then the value at 298.15 K is subtracted from the intermediate values, giving negative values for the enthalpy below 298.15 K.

The tables extend to well above the normal melting point to provide data in a metastable region which in this case is a superheated region. Explanations are inserted in the tabulations to indicate the end of the phase stability and any solid-state transitions.

Liquid Phase Thermal Functions

The construction of the liquid single-phase thermal functions is identical with that used for the solid phase; however, the required data at 298.15 K are not usually readily available. The data are obtained by calculating a preliminary table using the chosen heat capacities with zero values for $\Delta_f H^\circ$ (298.15 K) and S° (298.15 K). The correct starting values are then determined by comparing the values from the tables of crystal and liquid, using the following equations:

$$\Delta_{fus} H^\circ = \Delta_f H^\circ(T_{fus}, \text{l}) - \Delta_f H^\circ(T_{fus}, \text{cr}),$$

$$\Delta_{fus} S^\circ = \Delta_{fus} H^\circ / T_{fus} = S^\circ(T_{fus}, \text{l}) - S^\circ(T_{fus}, \text{cr}).$$

The correct values at 298.15 K may be obtained from the above relations. A typical liquid table is extrapolated both below the melting point (if the melting point is above 298.15 K) and above the boiling point to facilitate interpolation and to provide data in the metastable regions, both in the supercooled and superheated regions. A glass transition may be included in which case the tabulation becomes a multiphase table.

Gas Phase Thermal Functions

The gas phase thermal functions are generated using statistical mechanical relationships. Minimal data required for the various types of molecules are summarized below. Some of the equations used are given in Sec. 6.1 on Calculational Methods. The relative molecular mass is required for all molecules. Minimum information required is:

Monatomic species:
: Low-lying atomic energy levels and their statistical weights.

Diatomic species:
: Spectroscopic parameters such as the vibrational-rotational constants, symmetry number, and low-lying electronic energy levels.

Linear polyatomic species:
: Rotational constant, symmetry number, vibrational frequencies, and low-lying electronic levels.

Nonlinear polyatomic species:
: Principal moments of inertia, symmetry number, vibrational frequencies, and low-lying electronic levels.

Multiphase Tables

Tables which show only values for the stable phases at 1 bar pressure are multiphase tables. Multiphase tables can always be recognized by the presence of solid lines, indicating phase transitions, on the table. They are prepared in a manner similar to tables for condensed phases. The functions are evaluated in the same manner as for a solid up to the first transition point; then the enthalpy and entropy of transition are added and the integration is continued using the heat capacities of the next phase. At each transition, the above process is repeated.

6.1. Calculational Methods

The calculation of the temperature-dependent values of the thermal function is performed using a variety of procedures. Some of these procedures were developed internally while others were developed at other locations. A general description of the traditional equations used in the JANAF project follows. Numerous higher order calculational schemes are used whenever the data are sufficient. These procedures are detailed on the appropriate tables.

In gas phase calculations, all thermodynamic variables are calculated in dimensionless form, e.g., C_p/R to at least seven significant figures. This is an arbitrary choice since most data do not warrant this accuracy. This has been done to permit the calculation of the crossover temperatures and enthalpies between single-phase tables accurately and to permit conversion to the desired units without loss of accuracy. The printed tables, however, will only contain three decimal places. Condensed phase tables do not depend directly on R (the gas constant) and they are not calculated in dimensionless form, but are calculated to five decimal places for units conversion.

Condensed Phase Species

Thermodynamic data for condensed states are derived from either measured or estimated information. The thermochemical table is obtained normally by the appropriate integration of heat capacity data. At the. appropriate temperatures, transition enthalpies are added to the enthalpy total, while the quotient of the transition enthalpy divided by the thermodynamic temperature is added to the entropy total.

Gaseous Species

Calculation of the contributions of rotation and translation involves the use of quantum statistics, but to obtain a numerical solution, the quantum statistics are usually replaced by classical statistics at temperatures above about 10 K; below 10 K this classical approximation no longer holds. For this reason the equations presented here fail in the vicinity of $T \rightarrow 0$. In agreement with the third-law concept, C_p° and S° are zero at $T \rightarrow 0$. For a reference element, $\log K_f$ is zero at $T \rightarrow 0$, while for compounds the absolute values of the Gibbs energy function and $\log K_f$, become infinite at $T \rightarrow 0$, for the choice of the enthalpy reference temperature of 298.15 K.

In addition, classical statistics can sometimes lead to erroneous results at high temperatures. For example, the classical approximation could give abnormally high C_p° values for a diatomic molecule having a shallow potential energy curve.

The functions calculated for gases are obtained, in general, from molecular constants that have been adjusted to the natural isotopic abundance. Normally, the approximation of adjusting the molecular parameters by a weighting according to a weighted natural isotopic abundance can be made. The proper correction (which is used for all reference states) is based on a weighted isotopic average of the tabulations.

An electronic term of unit statistical weight lying at 30 000 cm^{-1} and above contributes a negligible amount to the thermodynamic functions at temperatures of 6000 K and below. On the other hand, a number of such terms cannot be neglected. In these cases, the number of terms and their values have been summed and their contribution included.

Some fundamental vibrational frequencies have been estimated by analogy with related molecules. Occasionally, two or more fundamentals are estimated at the same value. This is not to be confused with a true degeneracy which is indicated by placing the degeneracy value in parentheses following the frequency. However, when the information has been taken from another compilation, the degeneracies indicated by the compiler have been retained.

The method used in generating the thermal functions depends not only on the quality/quantity of information available but also on the specifics of the nature of the information (e.g., split ground state, shallow potential wells, etc.). The gas phase tables are generated using the following relationships unless stated otherwise. These relationships are given in Mayer and Mayer[30] and Pitzer and Brewer.[31]

Use of a more sophisticated approach will always be noted and details given on the appropriate tables. The more common alternative approaches are given by McBride and Gordon[32] and McDowell[33] for monatomic and polyatomic gases. For many diatomic gaseous molecules (the alkali metal dimers, the alkaline earth metal dimers, the halogens, hydrogen, deuterium, nitrogen, oxygen, sulfur), a direct summation technique has been used. This technique, stated explicitly on the individual tables, involves a summation over the individual rotation-vibrational energy levels for each electronic state in the partition function expression. In addition, the summation is terminated at the dissociation energy for a particular electronic state of the diatomic molecule; although in some cases, the metastable states (above the dissociation energy) are included in the summation.

6.1.1. Ideal Monatomic Gas

(a) Translation

$$C_p^\circ/R = 5/2,$$

$$[H^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = 5/2$$

$$S^\circ/R = 3/2 \ln M_r + 5/2 \ln T + 5/2 + \ln \frac{k}{p^\circ}\left(\frac{2\pi k}{Nh^2}\right)^{3/2},$$

$$-[G^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = 3/2 \ln M_r + 5/2 \ln T + \ln \frac{k}{p^\circ}\left(\frac{2\pi k}{Nh^2}\right)^{3/2}.$$

(b) Electronic

$$C_p^\circ/R = T^2\frac{d^2\ln Q}{dT^2} + 2T\frac{d\ln Q}{dT}$$

$$[H^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = T\frac{d\ln Q}{dT^2},$$

$$S^\circ/R = T\frac{d\ln Q}{dT^2} + \ln Q,$$

$$-[G^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = \ln Q,$$

where

$$Q = \sum_i g_i \exp(-c_2\epsilon_i/T),$$

where ϵ_i is in cm^{-1} and the electronic levels to be included are discussed on the appropriate gas phase table.

6.1.2. Ideal Diatomic Gas

(a) Translation: Same as in I(a).

(b) Rotation

$$C_p^\circ/R = 1 + (c_2B/T)^2/45,$$

$$[H^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = 1 - (c_2B/T)/3 - (c_2B/T)^2/45.$$

$$S^\circ/R = 1 - \ln(c_2B\sigma/T) - (c_2B/T)/90.$$

$$-[G^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = -\ln(c_2B\sigma/T) + (c_2B/T)/3 + (c_2B/T)^2/90,$$

where

$$B = (B_e - \alpha_e/2);$$

in cm^{-1} when spectroscopic constants are available, or

$$B = h/8\pi^2cI = 2.799\,320 \times 10^{-39}/I;$$

in cm^{-1} when calculated from molecular model, I in $g\cdot cm^2$.

(c) vibration

$$C_p^\circ/R = u^2e^{-u}/(1 - e^{-u})^2,$$

$$[H^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = ue^{-u}/(1 - e^{-u}),$$

$$S^\circ/R = ue^{-u}/(1 - e^{-u}) - \ln(1 - e^{-u}),$$

$$-[G^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = -\ln(1 - e^{-u}),$$

where

$$u = c_2(\omega_e - 2\omega_e x_e)/T;$$

when spectroscopic constants (in cm^{-1}) are available, or

$$u = c_2\omega/T;$$

where ω (in cm^{-1}) is the fundamental frequency of a harmonic oscillator.

(d) Corrections for anharmonic vibrations

$$C_p^\circ/R = \frac{16\gamma}{u} - \frac{\delta u^2e^u}{(e^u - 1)^2} + \frac{u^2e^u(2\delta e^u - 4Xu - 8x)}{(e^u - 1)^3} + \frac{12Xu^3e^{2\cdot u}}{(e^u - 1)^4},$$

$$[H^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = \frac{8\gamma}{u} + \frac{u(\delta e^u - 2X)}{(e^u - 1)^2} + \frac{4Xu^2e^u}{(e^u - 1)}$$

$$S^\circ/R = \frac{16\gamma}{u} + \frac{\delta}{(e^u - 1)} + \frac{\delta ue^u}{(e^u - 1)^2} + \frac{4Xu^2e^u}{(e^u - 1)^3},$$

$$-[G^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = \frac{8\gamma}{u} + \frac{\delta}{(e^u - 1)} + \frac{2Xu}{(e^u - 1)^2},$$

where $u = (\omega_e - 2\omega_e x_e)(c_2/T)$, $X = \omega_e x_e/\omega_e$, $\delta = \alpha_e/B_e$, and $\gamma = B_e/\omega_e$; ω_e, $\omega_e x_e$, B_e and α_e are in cm^{-1}.

(e) Electronic

Same as I(b) when the ith-state vibrational partition function, Q_v^i, and the ith-state rotational partition function, Q_r^i, are equal to the respective ground-state partition functions. In this case the partition function

$$Q = Q_tQ_vQ_r^i\sum_i Q_e^i,$$

otherwise all the thermodynamic functions are derived from

$$Q = Q_t^i\sum_i Q_e^iQ_v^iQ_r^i,$$

where Q_t is the translational partition function and

$$Q_e^i = g_i \exp(-c_2\epsilon_i/T).$$

6.1.3. Linear Polyatomic Molecule

(a) Translation: Same as in I(a).

(b) Rotation: Same as in II(b).

(c) Vibration: Same as in II(c) for $3N - 5$ vibrational degrees of freedom.

(d) Corrections for anharmonic vibrations: This contribution is normally neglected.

(e) Electronic: Same as II(e) where levels and quantum weights are known.

6.1.4. Nonlinear Polyatomic Molecule (Rigid Rotator, Harmonic Oscillator)

(a) Translation: Same as in I(a).

(b) Rotation:

$$C_p^\circ/R = 3/2,$$

$$[H^\circ(T) - H^\circ(0\,\mathrm{K})]/RT = 3/2,$$

$$S°/R = \frac{3}{2} + \frac{1}{2}\ln(I_A I_B I_C) - \ln\sigma + \frac{3}{2}\ln T + (-\frac{3}{2}\ln\frac{h2}{8R\pi°} + \frac{1}{2}\ln\pi)$$

$$-[G°(T) - H°(0\,K)]/RT = \frac{1}{2}\ln(I_A I_B I_C) - \ln\sigma + \frac{3}{2}\ln T + (-\frac{3}{2}\ln\frac{h2}{8R\pi°} + \frac{1}{2}\ln\pi)$$

(c) Vibration
Same as II(c) for $3N - 6$ vibrational degree of freedom.

(d) Corrections for anharmonic vibrations.
This contribution is normally neglected.

(e) Electronic
Same as II(e) where levels and quantum weight are known.

6.2. Dates

At the bottom of the tabulation side of each table, there are one or two dates. These dates refer to the approximate time at which the evaluation for these tables was completed. The data for the most recent and the preceding evaluation are given. These dates will be at the bottom of the page at the right-hand side and left-hand side, respectively. Previously, all revision dates had been listed. Current practice will limit the dates to two. For the gas phase tables, the standard-state pressure is given in parentheses after the date(s). If the dates are identical, then the difference in this current table and its predecessor lies in the changes due to the standard-state pressure. Contrary to previous practice, the latest issue date of each table is not given in either of the two indices in this publication.

7. Additions, Revisions, and Corrections

In this Fourth Edition there are numerous typographical errors from the Third Edition which have been corrected. However, there are calculation errors in the formation properties for the following compounds: $AlCl_4Na$(cr), BHO_2(cr), BH_2O_2(g), $B_8K_2O_{13}$(l), Be_4O_4(g), Br_3OP(g), Br_3PS(g), CH^+(g), CN(g), CO(g), CTi(cr), C_2H_2(g), C_2Li_2(cr), C_2Mg(cr), CH_3Cl_3Si(g), CH_3F_3Si(g), ClFMg(g), ClH_4N(cr), Cl_4Mo(g), Cl_4Pb(g), Cl_4Ti(cr, l, cr/l), F_2Hg_2(cr), F_2Ti(g), FeH_2O_2(g), HP(g), HS(g), H_2P(g), H_3P(g), Hg^+(g), LiO^-(g), $Mg_3P_2O_8$(cr), OS_2(g), W(g), W^+(g), Zr(g), and Zr^+(g). These also have been corrected.

In addition new tables have been constructed many halogen oxides. These include 5 iodine oxides, 5 bromine oxides, 7 chlorine oxides, and 4 oxygen fluorides.

8. Acknowledgments

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10. Indices to Tables

There are two indices provided with this publication. Both indices are alphabetical, one by chemical name and one by chemical formula. In both cases the state of the compound is given in parentheses after the chemical formula. The tables and discussions are arranged in the same order as given in the chemical formula index.

10.1. Description of the Chemical Formula Index to the NIST-JANAF Thermochemical Tables

The tables included in this publication are ordered as given by the Chemical Formula Index. The modified Hill indexing system [J. Am. Chem. Soc. **22**, 478 (1900)] for chemical compounds, as used by Chemical Abstracts, is employed here to order the tables.

The Hill empirical formula is obtained for a particular compound by placing the elements in their alphabetical order unless C is present, in which case C is placed first, H second, and the remaining elements in alphabetical order. Substances with the same Hill formula are ordered alphabetically by their name. However, tables representing different states of the same species are in the order crystal, liquid, crystal-liquid, and ideal gas.

As examples, BeCl(g) would appear as written, whereas NaCl(g) would be filed under ClNa(g). To expand on the ordering of carbon compounds, the C always comes first, followed immediately by H if hydrogen is present, and then followed by any other elements present in their normal alphabetical order. The number of atoms of the element indexed first also influences the order of indexing the compound; e.g., all formulas with C (one carbon atom only) come before those with C_2 (two carbon atoms), followed by C compounds, and so on. Thus: $CHBF_4O$ (formyl fluoride, compound with BF_3), $CHCl_3$ (chloroform), CH_2F_3P (trifluormethylphosphine), CH_3NO_3 (methyl nitrate), CH_4C1_2Si (dichloromethylsilane), $CH_{10}N_4O_3$ (hydrazine carbonate), CO (carbon monoxide), CO_2 (carbon dioxide), CO_3Zn (zinc carbonate), CZr (zirconium carbide), C_2Ba (barium acetylide), C_2BrClF_2 (bromochlorodifluoroethylene), C_2Ca (calcium carbide), and so on. See any formula index of Chemical Abstracts for further details and examples.

The electron gas, e^- (ref st), is inserted in the filing order after the deuterium species. Nonstoichiometric compounds are inserted just prior to or just after the corresponding stoichiometric order.

10.2. Description of the Chemical Name Index to the NIST-JANAF Thermochemical Tables

The nomenclature for the chemical species included in this publication does not fully correspond to the current Chemical Abstracts practice. The attempt has been made to use names as easily understandable as possible while not deviating far from the Chemical Abstracts system. Cited are two examples where the Chemical Abstracts nomenclature is followed, $AlBr_3$(g) and BBr_3(g) are listed as aluminum bromide and tribromoborane, respectively. For historical reasons, we would have preferred to name BBr_3(g) as boron bromide. However, Chemical Abstracts refers to most boron halides as borane derivatives. On the other hand, whereas Al_2Br_6 is called di-μ-bromotetrabromoaluminum in Chemical Abstracts, this publication uses aluminum bromide.

In summary, general comments on the nomenclature are:

(1) The carbon and silicon neutral species follow the Chemical Abstracts organic-type nomenclature in which the name reflects the type of bonding.

(2) The -ium suffix that denotes positive ions is not used. CH^+(g) is named 'methylidyne, ion' whereas Chemical Abstracts uses methyliumylidene.

(3) Salts are not named as an acid, metal salt of. For example, $BaSO_4$ is barium sulfate, not sulfuric acid, barium salt.

(4) Many mineral names are used.

(5) The sometimes confusing nomenclature for bridged structures in dimers is not used. Normally the monomer name is used.

In adopting this modified Chemical Abstracts nomenclature, there are numerous species for which the name will be significantly different from earlier JANAF publications. It is impractical to list all name changes, but in the more severe cases, a comment is made on the tables as to the previously used name.

10.3 Chemical Formula Index

10.4 Chemical Name Index