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EVALUATION AND COMPILATION OF THERMODYNAMIC PROPERTIES
OF HIGH TEMPERATUR (U) DOW CHEMICAL CO MIDLAND NICH
THERMAL RESEARCH LAB M W CHASE 13 AUG 87

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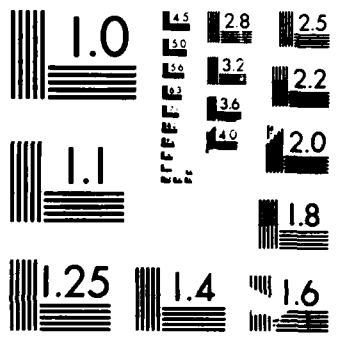
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MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS 1963-A

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19. ABSTRACT (Continue on reverse if necessary and identify by block number) This work involves a continuing effort to provide a set of critically evaluated, internally consistent, high temperature thermochemical tables; the JANAF Thermochemical Tables. During this contract period, the chemical species studied fell into three categories - alkaline earth species, alkali metal species, and elements. The species in the alkaline metal series include the metals themselves, hydroxides, halides, oxides, sulfides, sulfates and carbonates. The species in the alkali metal series include the halides and the carbonates. The elements under study include boron and aluminum. The support information gathered for the study of these chemical species has been collected together in a concise readable form and is available upon request. The calculation of the thermodynamic functions for diatomic gases was greatly enhanced by the addition of two calculational techniques. These procedures permit a more accurate accounting of the vibrational-rotational energy levels for each electronic state, including the metastable levels just above the dissociation limit. These procedures are particularly			
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important in those cases where the electronic potential energy curve is very shallow,
i.e. diatomic beryllium *Keywords*

During this contract period, this project was transferred from the Dow Chemical Company
to the U.S. National Bureau of Standards.

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FINAL REPORT

20 May 1985 to 19 May 1986

**Evaluation and Compilation of Thermodynamic Properties
of High Temperature Chemical Species**

under Contract F49620-85-C-0076

with The Dow Chemical Company

Midland, Michigan 48674

Dr. M. W. Chase, Principal Investigator

Sponsored by

Air Force Office of Scientific Research

Air Force Systems Command

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INTRODUCTION

The JANAF Thermochemical Tables provide the United States Air Force and its contractors with critically evaluated thermodynamic data. The tables, issued as quarterly supplements, are a collection of loose-leaf pages which allow easy updating. The updating, either by revision of old tables or addition of new tables, is dictated by current and anticipated future needs of the United States Air Force. Each table contains not only a temperature-dependent set of seven thermodynamic functions but also a critical discussion of the relevant literature on which the thermodynamic values are based.

The distribution of the JANAF quarterly supplements during this contract period was complicated by the simultaneous preparation of the Third Edition of the JANAF Thermochemical Tables. This hard bound book is a rewriting of the the tables in a consistent format with a concurrent recalculation of all tabulations in terms of the current values of the fundamental constants, relative atomic weights, and the thermodynamic properties of the reference elements. This rewriting should not be confused with a re-analysis of all tabulations. The Third Edition, to be published in SI units (i.e., Joules, rather than calories) will contain more temperature dependent information than previous publications.

The prime goal of this contract has been to critically evaluate and compile a high quality self-consistent set of tables of thermodynamic properties. At the same time, a secondary effort has been expended to maintain and make available, in an easily readable form, all information collected during the evaluation process. This would include the literature citations for all article consulted, lists of all experimental and theoretical data examined, and comments as to the need of additional information.

This evaluation effort necessitated the collection and critical reading of numerous articles from the literature. Each article required extensive analysis to measure the reliability of the results. By having a compilation center perform this task, the Air Force is assured of increased internal consistency in the tabulations. In turn, the Air Force can better redirect its efforts to evaluate the reliability of "products" which depend on this thermodynamic data.

This contract work provides a compact, consistent, and well documented set of thermodynamic values. By consolidating such activity, Air Force personnel do not have to rely on their own personal efforts to produce the necessary tabulations for their research and development. This reduces duplication of effort within the Air Force in the area of high temperature thermodynamic properties of chemical species. In fact, it has resulted in an exchange of information and substantial cooperation.

During this contract period, the principal investigator, Dr. Malcolm W. Chase, transferred to the U. S. National Bureau of Standards. Thus, the day to day operation as of February, 1986 was continued at this new location. All support

information (computer programs and files, literature files, and the notes on all JANAF activities) was transferred to the Gaithersburg, Maryland site.

Work covered under contract No. F49620-85-C-0076 has been performed by Malcolm W. Chase, David J. Frurip, Joseph R. Downey, Jr., Richard A. McDonald, and Alan N. Syverud. Extensive clerical help at The Dow Chemical Company was provided by Ann Schmidt, Jan Crouch, Betty Clark, Rhoda Toth, Barbara Meier, and Jackie DeLong. Considerable technical assistance was provided by Milton. D. Marks. Program coordination and direction during the performance of the contract has been provided by Dr. Leonard H. Caveny, Directorate of Aerospace Science, AFOSR.

CURRENT STATUS OF JANAF THERMOCHEMICAL TABLES

During this contract period, the JANAF Thermochemical Tables were undergoing a complete rewriting in order to publish a hard bound book (with financial assistance from the Department of Energy). This publication was to contain tabulations up to and including the supplement dated September, 1984. Additional species, i. e. those contained in supplements dated December 1984 to June 1986 will be collected together to be published after the distribution of the Third Edition of the JANAF Thermochemical Tables.

During this contract period, many elements were re-examined and reissued. Also of interest was the examination of the alkali metals oxides, halides, and carbonates. Particular emphasis was directed towards potassium chloride in order to better appreciate the effort necessary to examine the alkali metal halides. The presumed difficulty lies in the fact that the vapor phase contains dimeric species. A cooperative venture was undertaken here as there were three other groups interested in the thermodynamic description of potassium chloride. These groups were: U. S. National Bureau of Standards, U. K. Atomic Energy Research Establishment, and the Institute of High Temperatures (U.S.S.R.). A continued effort was directed at the completion of the alkaline earth species.

NEW APPROACHES IMPLEMENTED DURING THE CONTRACT PERIOD

1. The monatomic gas partition function calculation was re-examined so as to incorporate the recent contribution of K. S. Pitzer (J. Chem. Phys. 70, 393 [1979]). It was necessary to evaluate this method as to its possible adoption as the preferred method for the calculation of the thermal functions for monatomic gases.
2. With the assistance of F. M. Mies and P. S. Julienne (J. Chem. Phys. 77, 6162 [1982]), a considerably improved treatment of the energy levels in a diatomic system is possible. This approach and a direct summation technique (William H. Evans) have been used to evaluate the thermodynamic properties of the alkali metal dimers, the alkaline earth dimers, and the halogens.
3. The analysis of the Fe/O system will be available to the JANAF staff from Dr. John L. Haas, U. S. Geological Survey. Dr. Haas is using a simultaneous analysis approach (PHAS20 computer program) to evaluate hundreds of related studies involving wustite, magnetite, and hematite. The JANAF staff has been involved in the review of this work. The final results will be incorporated in the our publications. In addition, the PHAS20 program will be installed on the NBS computer system.

INTERACTIONS

During the course of this contract period, members of the JANAF staff attended two conferences: the Mid-West High Temperature Chemistry Conference (Iowa State University, 9-12 June 1985), and the 40th Calorimetry Conference (Asilomar, 25-29 August 1985).

The JANAF Thermochemical Tables project benefits yearly from innumerable discussions with scientist throughout the United States and even overseas. During the course of this particular contract period, the prime interactions occurred with Drs. D. L. Hildenbrand (SRI), F. L. Mies and P. S. Julliene (NBS), L. Brewer (Berkeley), M. H. Rand (Harwell), J. L. Haas (USGS), and the Chemical Thermodynamics Data Center at NBS.

PUBLICATIONS

This contract period produced four supplements. These would normally be distributed to a restricted mailing list (as provided by the AFOSR). Due to the impending publication of the Third Edition of the JANAF Thermochemical Tables, such distribution was withheld. This decision was made so as to avoid the delemma of having loose leaf tables in different units in the same loose leaf collection. Thus, these table will be distributed after the distribution of the Third Edition.

In addition to the loose-leaf supplements, there are a series of publically available publications which contain tables as follows: NSRDS-NBS-37 (5) contains all supplements up to and including No. 33; t.e 1974 Supplement (6) contains Nos. 34-37; the 1975 Supplement (7) contains Nos. 38-41, the 1978 Supplement (8) contains Nos. 42-45, and the 1982 Supplement (9) contains Nos. 46-52. These five publications should be used together as a complete set and are current as of June 30, 1978.

The Third Edition (10) supercedes all previous JANAF publications and contains all supplements up to and including the September 1984 supplement.

PUBLICATIONS LIST

1. JANAF Thermochemical Tables, PB 168370, Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, 1965.
2. JANAF Thermochemical Tables, PB 168370-1, Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, 1966.
3. JANAF Thermochemical Tables, PB 168370-2, Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, 1967.
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5. D. R. Stull and H. Prophet, Project Directors, JANAF Thermochemical Tables, 2nd Edition, NSRDS-NBS 37, Catalog Number C13.48:37, U.S. Government Printing Office, Washington, D.C., 1971.
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7. M. W. Chase, J. L. Curnutt, H. Prophet, R. A. McDonald, and A. N. Syverud, JANAF Thermochemical Tables, 1975 Supplement, J. Phys. Chem. Ref. Data 4, 1 (1975).
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9. M. W. Chase, J. L. Curnutt, J. R. Downey, R. A. McDonald, A. N. Syverud, and E. A. Valenzuela, JANAF Thermochemical Tables, 1982 Supplement, J. Phys. Chem. Ref. Data 11, 695 (1982)
10. M. W. Chase, C. A. Davies, J. R. Downey, D. J. Frurip, R. A. McDonald, and A. N. Syverud, JANAF Thermochemical Tables, Third Edition, J. Phys. Chem. Ref. Data 14, Supplement No. 1, 1985

CURRENT INDEX OF JANAF THERMOCHEMICAL TABLES

A complete listing, as of March 31, 1986, of the JANAF Thermochemical Tables is available upon request. This listing indicates those chemical species on which compilations were made during the present and prior contract periods, i.e. each tabulation and its most recent issuance date is given. This list currently contains approximately 1800 species.

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