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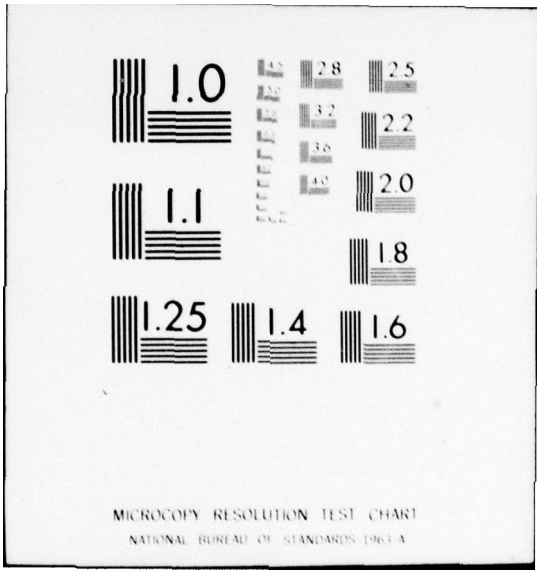
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This work involves a continuing effort to provide a set of critically evaluated, internally consistent, high temperature thermochemical tables: the JANAF Thermochemical Tables. In this three year contract period 147 revised and 152 new thermochemical tables were issued. A portion of these tables resulted from a concurrent Department of Energy contract. This brings the total number of JANAF Thermochemical Tables to 1449. In this contract period new reference states were issued for nickel, deuterium and the rare gases while reference states for hydrogen, fluorine, oxygen, nitrogen, and sulfur were revised. (cont)

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Numerous new or revised tables were issued dealing with the alkaline earth halides and hydroxides, zirconium tetrahalides, numerous aluminum and boron species, silicon halides, halogenated silanes, and fluorinated and deuterated species. The 299 thermochemical tables were issued as eight supplements (Nos 43-50) to the JANAF Thermochemical Tables. In addition, supplements 42-45 were combined in a minuscript to be published in J. Phys. Chem. Ref. Data in 1978. Calculational procedures for producing thermochemical tables of gas phase species were reviewed amd assessed for publication. These included extending monatomic gas calculations above 6000 K, implementation of a direct summation method for diatomic molecules, and the moment of inertia calculation for polyatomic molecules.

AFOSR-TR- 78-1060

FINAL REPORT

1 January 1975 to 31 December 1977

Evaluation and Compilation of Thermodynamic Properties of High Temperature Chemical Species

under Contract F44620-75-C-0048

with The Dow Chemical Company

Midland, Michigan 48640

Dr. M. W. Chase, Principal Investigator

Sponsored by

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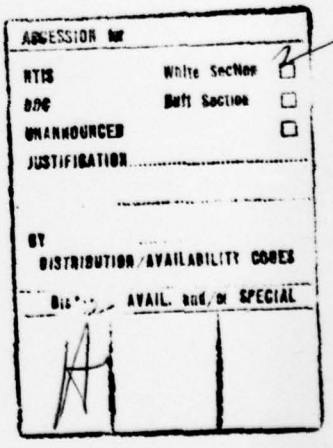

March 31, 1978

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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.

The goal of this contract has been to critically evaluate and compile a high quality self-consistent set of tables of thermodynamic properties. During the contract period, 299 tabulations have been issued. [Some of these tables were generated under a concurrent contract with the Department of Energy.] This effort necessitated the collection and evaluation 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 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.

Work covered under contract No. F44620-75-C-0048 has been performed by M. W. Chase, J. L. Curnutt, J. R. Downey, Jr., R. A. McDonald, A. N. Syverud, and E. A. Valenzuela. Program coordination and direction during performance of the contract has been provided by Dr. Joseph F. Masi, Directorate of Aerospace Science, AFOSR.

CURRENT STATUS OF JANAF THERMOCHEMICAL TABLES

The eight supplements (Nos 43-50) distributed in this contract period contained 299 tables for various chemical species. Of these, 147 (49%) were revised tables and 152 (51%) were new tables. This brings the total number of high temperature tables to 1449. [As mentioned earlier, a portion of these tables resulted from a concurrent Department of Energy contract.] New reference states include nickel and deuterium (the rare gases for the DOE contract) while revised reference states include hydrogen, fluorine, oxygen, and nitrogen (sulfur for the DOE contract).

The most significant results from the recent effort for AFOSR are the revisions and additions in the thermodynamic properties of the alkaline earth halides and hydroxides, zirconium tetrahalides, numerous aluminum and boron species, silicon halides and halogenated silanes. Fluorinated and deuterated species, originally compiled by the U. S. Bureau of Standards personnel, were also included.

NEW APPROACHES IMPLEMENTED DURING THE CONTRACT PERIOD

1. The monatomic gas partition function calculation was examined in light of possibly extending the tabulations to temperatures greater than 6000 K. The various methods available in the literature have been examined and summarized in a report by Joseph R. Downey, Jr.
2. With the assistance of William Evans (U.S. National Bureau of Standards) a direct summation technique was used to generate tables for $H_2(g)$, $D_2(g)$, and HD(g) and their unipositive ions. We have compared our results with those generated by a similar procedure used by L. V. Gurvich, and V. S. Yungman at the Institute of High Temperatures (Moscow). A similar study on $O_2(g)$ and $S_2(g)$ is proposed.
3. In the case of polyatomics, the aim is to better use the vibrational data available by current experimental techniques. This data provides quantitative evidence for departure from rigid rotator harmonic oscillator approximation. Programs written by B. J. McBride and S. Gordon and R. S. McDowell have been implemented to account for this departure. In addition the moment of inertia calculation has been upgraded to improve usefulness (report to be issued under auspices of a concurrent Department of Energy contract). A reinvestigation of internal rotation is also underway.
4. A highlight of the contract period is the extensive cooperation and data exchange which developed. The U.S. National Bureau of Standards, U.S. Geological Survey, and the Chemistry Departments of University of California at Berkely and Massachusetts Institute of Technology have extended considerable efforts which increase the efficiency and quality of our program.

PUBLICATIONS

The three year contract period produced eight supplements, Nos. 43-50, which were distributed to a restricted mailing list. To further increase the availability of the tables to the Air Force support community, we generated a publication (4) which combined supplement Nos. 42-45. Earlier publications in this series (1, 2, 3) are as follows: NSRDS-NBS-37 (1) contains all supplements up to and including No. 33; the 1974 Supplement (2) contains Nos. 34-37; and the 1975 Supplement (3) contains Nos. 38-41. These four publications should be used together as a complete set and are current as of June 30, 1976. For completeness, all the JANAF Thermochemical Tables publications (1-8) are listed on the following page.

In addition, two other publications were issued in this contract period (9, 10). In his critical evaluation of data for the aluminum oxides, Alan N. Syverud also studied the boron-oxides in hopes of establishing thermochemical similarities. As a result, an article (9) on the molecular structure of $B_2O_2(g)$ and $Al_2O_2(g)$ was published in response to a similar article which appeared in the literature in 1976. A second publication (10) by Joseph R. Downey, Jr. summarizes the alternative calculational procedures for monatomic gas partition functions and discusses the adopted JANAF procedures.

To promote discussion and further specific experimentation, two talks were given by Alan N. Syverud at two Midwest High Temperature Chemistry Conferences. These talks dealt with family trends in the properties of the alkaline earth oxides and monohalides. Discrepancies and areas needing further study were emphasized.

Publications

1. JANAF Thermochemical Tables, 2nd Edition, NSRDS-NBS-37, Catalog Number C13.48:37, U.S. Government Printing Office, Washington, D.C., 1971.

2. JANAF Thermochemical Tables, 1974 Supplement, J. Phys. Chem. Ref. Data 3, 310 (1974).

3. JANAF Thermochemical Tables, 1975 Supplement, J. Phys. Chem. Ref. Data 4, 1, (1975).

4. JANAF Thermochemical Tables, 1978 Supplement, J. Phys. Chem. Ref. Data, Vol. 7, No. 3, 1978; to be published.

5. JANAF Thermochemical Tables, PB 168370, Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, 1965.

6. JANAF Thermochemical Tables, PB 168370-1, Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, 1966.

7. JANAF Thermochemical Tables, PB 168370-2, Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, 1967.

8. JANAF Thermochemical Tables, PB 168370-3, Clearinghouse for Federal Scientific and Technical Information, Springfield, Virginia, 1968.

9. A. N. Syverud, "Molecular Structure of B_2O_2, Al_2O_2, and other Chalcogenides of the Aluminum Family", J. Inorg. Nucl. Chem. 38, 2163 (1976).

10. J. R. Downey, Jr., "Calculation of Thermodynamic Properties of Ideal Gases at High Temperatures: Monatomic Gases", to be published as AFOSR Technical Report, 1978.

CURRENT INDEX OF JANAF THERMOCHEMICAL TABLES

A complete listing, as of December 31, 1977, 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.