NATIONAL BUREAU OF STANDARDS REPORT

7587

PRELIMINARY REPORT
ON THE THERMODYNAMIC PROPERTIES OF
SELECTED LIGHT-ELEMENT AND
SOME RELATED COMPOUNDS

(Supplement to NBS Reports 6297, 6484, 6645, 6928, 7093, 7192, and 7437)

1 July 1962

NBS

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

THE NATIONAL BUREAU OF STANDARDS

Functions and Activities

The functions of the National Bureau of Standards are set forth in the Act of Congress, March 3, 1901, as amended by Congress in Public Law 619, 1950. These include the development and maintenance of the national standards of measurement and the provision of means and methods for making measurements consistent with these standards; the determination of physical constants and properties of materials; the development of methods and instruments for testing materials, devices, and structures; advisory services to government agencies on scientific and technical problems; invention and development of devices to serve special needs of the Government; and the development of standard practices, codes, and specifications. The work includes basic and applied research, development, engineering, instrumentation, testing, evaluation, calibration services, and various consultation and information services. Research projects are also performed for other government agencies when the work relates to and supplements the basic program of the Bureau or when the Bureau's unique competence is required. The scope of activities is suggested by the listing of divisions and sections on the inside of the back cover.

Publications

The results of the Bureau's research are published either in the Bureau's own series of publications or in the journals of professional and scientific societies. The Bureau itself publishes three periodicals available from the Government Printing Office: The Journal of Research, published in four separate sections, presents complete scientific and technical papers; the Technical News Bulletin presents summary and preliminary reports on work in progress; and Basic Radio Propagation Predictions provides data for determining the best frequencies to use for radio communications throughout the world. There are also five series of nonperiodical publications: Monographs, Applied Mathematics Series, Handbooks, Miscellaneous Publications, and Technical Notes.

A complete listing of the Bureau's publications can be found in National Bureau of Standards Circular 460, Publications of the National Bureau of Standards, 1901 to June 1947 ($1.25), and the Supplement to National Bureau of Standards Circular 460, July 1947 to June 1957 ($1.50), and Miscellaneous Publication 240, July 1957 to June 1960 (Includes Titles of Papers Published in Outside Journals 1950 to 1959) ($2.25); available from the Superintendent of Documents, Government Printing Office, Washington 25, D. C.

NATIONAL BUREAU OF STANDARDS REPORT

NBS PROJECT		NBS REPORT
0300-11-03419 0302-11-03426 0307-11-03471 0501-11-05496 0903-11-09430 1501-11-15513 1504-11-15491	1 July 1962	7587

PRELIMINARY REPORT
ON THE THERMODYNAMIC PROPERTIES OF SELECTED LIGHT-ELEMENT AND SOME RELATED COMPOUNDS

(Supplement to NBS Reports 6297, 6484, 6645, 6928, 7093, 7192, and 7437)

Eighth Technical Summary Report
to the Advanced Research Projects Agency
on the Thermodynamic Properties
of Light-Element Compounds

Reference: ARPA Order No. 20-62

NBS

U. S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

ABSTRACT

This is the eighth semi-annual report on the current experimental, theoretical, and evaluative program, at the National Bureau of Standards, on the thermodynamic properties of selected light-element (and a few other) compounds of primary interest in high-temperature research. In this connection the chemical elements whose compounds are of greatest interest are considered to be H, Li, Be, B, C, N, O, F, Al, Cl, and Zr. The elements whose compounds are of secondary interest in the program are Mg, Si, K, Ti, Br, I, W, Hg, and Pb. The NBS work has emphasized the simpler compounds of these elements, but has included a number of compounds containing two of the metals named. The accomplishments of the various NBS groups in the program during the past year and their research plans during the coming year are discussed in Part A of the report.

The new NBS experimental results (presented in Part B) include the heat capacity and absolute entropy of aluminum carbide at low temperatures, and the heat capacity of beryllium nitride and beryllium aluminate at high temperatures (up to 1200°K), with resulting tables of thermodynamic functions. The experimental procedures of fluorine-combustion calorimetry described in detail gave as their best value a heat of formation of solid aluminum fluoride of $\Delta Hf^{o}_{298} = -358.3 \pm 0.3$ kcal/mole. Several techniques being used or developed for studying high-temperature vaporization in the Be-O-F and Al-O systems are extensively described, and early data and observations are presented.

Recent literature surveys included cover references on the heats of formation of compounds of 19 elements, as well as structure data on several alloy systems containing Be, Mg, Al, Zr, and/or W. Tables of the thermodynamic functions of 23 compounds containing Li, Mg, Al, Si, Ti, W, and/or Pb are given as the result of a detailed analysis of their published condensed-phase heat capacities. Similar tables resulting from new NBS spectroscopic data are given for the gas NF_2H and its isotopic analog NF_2D. The equilibrium pressures of the gases BeF, AlF, AlCl, and $AlCl_2$ under a variety of conditions and alternative assumed dissociation energies were calculated, and are presented graphically. The widely discrepant values that have been proposed for the dissociation energy of BeF are examined critically, with the conclusion that 8 electron volts is unreliable and that the true value is not far from 6 electron volts.

Thomas B. Douglas

Thomas B. Douglas, Project Leader

Chas W Beckett

Charles W. Beckett
Assistant Division Chief for Thermodynamics
Heat Division

TABLE OF CONTENTS

TABLE OF CONTENTS (continued)

TABLE OF CONTENTS (continued)

TABLE OF CONTENTS (continued)

TABLE OF CONTENTS (continued)

(Continued on next page)

TABLE OF CONTENTS (continued)

PART A. SUMMARY OF RESEARCH ACCOMPLISHMENTS AND PLANS FOR FUTURE WORK

INTRODUCTION

The NBS program has concentrated very largely on providing a complete and reliable set of thermodynamic properties for all substances which are, or are likely to be, important as products of combustion in chemical propulsion. This work has comprised two concurrent phases: (a) collecting and evaluating the results of published research, to establish already existing satisfactory values and to find where new values are needed, and (b) measuring new accurate data where needed, either with existing or with newly developed apparatus.

Phase (a) is now complete except for keeping abreast with current publications and using them to construct new or revised tables of thermodynamic properties. (Eventually the critical data assembly will be consolidated and issued as a formal publication.) During the past year the Bureau's work in this program has concentrated very largely on phase (b); while some new apparatuses are complex and are still in the development or the testing state, most are now sufficiently operational to yield new data.

In view of the practical goal stated above, the NBS program is largely limited to the simpler compounds of certain light elements. The experimental measurements give highest priority to compounds of Be, Al, Li, H, F, Cl, O, N, and C. The major emphasis during the present year's work and that planned for the next fifteen months is on compounds of beryllium and aluminum. Likewise, attention is being directed to include compounds of "mixed" type (e.g., ones containing two metals such as Be and Al, or two non-metals such as O and F).

A broader as well as more detailed statement of the general NBS program of measuring and evaluating the thermodynamic properties of light-element compounds is to be found in last summer's report (NBS Report 7192, 1 July 1961, pp. 1-5). A large number of specific substances were discussed there in terms of (a) their relative importance in chemical propulsion, (b) the adequacy or inadequacy of our knowledge of their thermodynamic properties, and (c) NBS plans for future work to help fill the most urgent data gaps—all as they appeared a year ago. Inevitably, certain changes in this status have occurred during the past year: practical priorities have changed somewhat, new data and data analyses have emerged from numerous organizations (including the National Bureau of Standards), and research along particular lines has moved faster or more slowly than then anticipated.

Following is a rather detailed account of what each NBS group in the program has accomplished during the past year and what it plans and expects to accomplish during the next year or fifteen months. In many of these discussions it has appeared desirable not to repeat extensive details of the methods pursued, since these remain largely the same and have been previously described in considerable detail (NBS Report 7192, pp. 6-22, and other semiannual reports under this program).

1. THERMOCHEMISTRY

Experimental Thermochemistry

The measurement of the heat of hydrolysis of nitronium perchlorate has been completed and a publication describing the work has been submitted to the NBS Journal of Research. Work has started on the measurement of the heat of solution of $BeCl_2$. The first set of measurements has indicated the probable existence of some impurity, probably moisture, in the sample. Because of the very large heat of reaction with water, steps to improve the sublimation and sample-transferring techniques have been taken. New samples will be prepared and the heat of solution measured. Crystallographic measurements will also be made to establish the crystal modification formed in the sublimation process.

Future plans for this program include measurements of the heat of formation of aluminum borohydride and hydrazine diperchlorate, using hydrolysis and solution reaction techniques if possible. We shall also undertake to measure the heat of formation of beryllium oxide using combustion calorimetry.

Tables of Thermodynamic Properties

The data on the heats of formation of a number of simple inorganic hydrides and oxidizers were reviewed and "best" values of the heats of formation were selected. The corresponding data on entropies and free energies for these substances will be reviewed during the coming year and "best" values of the free energies of formation will be selected.

A review of the data on heats of solution and dilution for aqueous solutions of some of the light element halides, nitrates, and other salts has been completed. These data will be combined with appropriate other data to yield values of the entropies of the aqueous ions.

2. FLUORINE COMBUSTION CALORIMETRY

During the past year the major accomplishment has been the completion of the experimental study of the heat of formation of AlF_3. This work is described in detail in a chapter of part B of this report. The final year of the study involved examination of the purity of the aluminum which had been burned, a study of the calibration of the calorimeter to improve the consistency of the calibration by various methods, and all the final series of measurements of the heat of combustion of teflon and of teflon-aluminum mixtures.

Preparations for the combustion of beryllium in fluorine, for the determination of the heat of formation of BeF_2, were initiated. The preparations have been more extensive than at first contemplated and have been carried out in order to reduce the hazard of contamination of instruments by BeF_2 which will be formed as a fine powder in the combustion. Pains have also been taken to reduce hazard to personnel. The preparations have included outfitting a dust enclosure for work with the calorimeter bomb before and after experiments and the handling of the products of combustion, a new fluorine handling manifold, and some adjustments to the calorimeter to reduce the extent of parts replacement and cleanup in event of accidental escape of soluble beryllium salts from the bomb.

A detailed summary covering about one year was made of the literature on the heats of formation of the compounds of interest to the program, and is included as chapter B1 of the previous semi-annual report (NBS Report 7437, January 1, 1962). A similar summary has been prepared for the first six months of 1962 and is included as a chapter of Part B of this report.

Plans for the Next Fifteen Months

Experimental combustions of beryllium in fluorine are expected to begin within the next quarter. Heat measurements on the formation of beryllium fluoride will then be made. Characterization of the product of combustion is an important step in this process, because the product of combustion will probably be microcrystalline or amorphous BeF_2. Determination of the heats of solution of the product of combustion and of macrocrystalline BeF_2 will probably be necessary for the characterization.

Studies of the heats of formation of Be_3N_2, Be_2C, Be_2B and Al_4C_3 will be carried out to the extent possible with the time and personnel available, using the fluorine combustion technique. No serious difficulty is expected in applying the technique to these compounds. The procurement of samples of adequate purity and their characterization is expected to be the major problem in their study.

If suitable personnel can be secured for the work a study, using the flame calorimeter, of the heat of formation of ClF_3 will be undertaken. For this experiment, the reaction of hydrogen gas with chlorine trifluoride gas is being considered, and would be carried out in a flow calorimeter.

3. LOW-TEMPERATURE CALORIMETRY

The low-temperature heat-capacity phase of the program is concerned with accurate measurements of the heat capacity from about 15° to 400°K and with calculations of the thermal functions from the data. These low-temperature measurements are coordinated whenever possible with the high-temperature relative-enthalpy investigations being carried out by another group in the program. Whenever applicable and practical the two groups investigate the same sample. The data from these two groups are combined to calculate thermal functions over the complete temperature range of measurements. Judicious extrapolation of the temperature range is made wherever possible or desirable. High-speed digital computer programs have been developed for analysis of the experimental data taken in the laboratory and for analysis of the literature data. Improvements are being made on these computer programs, also new computer programs are being developed as different requirements arise. Compilation and critical analysis of the original literature data are being made of substances that are of interest to the program and tables of thermal functions calculated. Improvements and extensions are made to existing compilations.

Heat-capacity measurements on both $LiAlH_4$ and LiH have been completed and preliminary values of thermal functions calculated assuming the samples that were investigated to be 100 percent pure. The samples contain, however, some impurities and these values of thermal functions must be adjusted accordingly. Chemical analyses requested from another group in the Bureau are expected to be completed in the near future.

Heat-capacity measurements on Al_4C_3 have been completed and the thermal functions calculated. The enthalpy change between 273.16° and 373.16°K (2933 cal/mole) derived from the measurements agrees within 0.2 percent of the average value (2939 cal/mole) obtained by another group in their relative enthalpy measurements (see NBS Report 7437, p. 17). The average deviation of their measurements was 0.6 percent. The two sets of data were combined, and thermal functions up to 2000°K were calculated. Details of this work are given in another section (Part B) of this report. In connection with the analysis of these data the IBM 704 computer programs were converted to that of the newly installed IBM 7090 computer. Programs used for analyzing literature data were also converted to programs compatible with the IBM 7090 computer.

Efforts to purify $AlCl_3$ by vacuum sublimation have failed thus far because of several breakages in the glass apparatus used. Apparently the $AlCl_3$ collected in compacted solid form in the first sublimation expanded sufficiently to break the glass receiver when subsequently heated for the second sublimation. Literature information seems to indicate that solid $AlCl_3$ has a large thermal expansion coefficient. The results of the work indicate that the sublimate should be collected as a powder to avoid the breakage through solid expansion. This will require a carrier-gas method instead of the vacuum method so that the material could be cooled readily into a powder before a compacted solid is formed. This work has been postponed temporarily to carry out heat-capacity measurements on other substances.

Some effort has been applied in the procurement of samples of interest to the program. Suppliers of metal carbides, nitrides, and borides and of binary metal oxides have been located, and orders for some of the substances have been made.

Literature surveys have been made on low-temperature heat capacity and entropy at 298.15°K of binary metal oxide compounds of Li, Be, Mg, Al, Si, K, Ti, and Zr and of elemental Si and K and some of their compounds (NBS Report 7437). Tables of thermal functions up to high temperatures are given in Appendix B of this report for some of the binary metal oxide compounds. Details of the data analysis to obtain the thermal functions are given in another section of this report (Part B).

The low-temperature heat capacity and, wherever available, high-temperature relative enthalpy data have been analyzed and thermal functions calculated for W, WO_2, WO_3, $MgWO_4$, Li_2TiO_3, $MgSiO_3$, Mg_2SiO_4, $MgTiO_3$, $MgTi_2O_5$, Mg_2TiO_4, Pb, PbO (yellow and red), PbO_2, Pb_2O_3, Pb_3O_4, $PbSiO_3$, Pb_2SiO_4, Al_2SiO_5 (andalusite, kyanite, and sillimanite), $BeSiO_4$, and Al_2TiO_5. Details of this analysis are given in another section of this report (Part B).

During the next fifteen months heat-capacity measurements already started on Be_3N_2 will be completed. Measurements on $Al_2O_3 \cdot BeO$ are expected to start soon. Depending upon the difficulties that might be encountered, about four to six of the following substances are planned for investigation.

a) $\underline{Be_2C}$

This substance now on order is expected to be delivered within the next few weeks.

b) $\underline{BeF_2}$

A high-purity sample in the glass state is on order. A sample of BeF_2 initially in the glass state was found by x-ray analysis to become highly, if not completely crystalline when annealed for 12 hours at 400°C. Additional annealing, if needed, should increase the crystallinity.

c) $\underline{Li_3AlF_6}$

It is hoped that a sample of this material may be made available in the near future.

d) Li_2BeF_4

Similar to Li_3AlF_6, a sample is scheduled for preparation by another government agency.

e) BeO

A sample that has been melted in an arc was recently received. The sample appears somewhat gray. The nature of the gray coloration is at present being investigated. The sample is expected to have considerably larger crystal size than the sample previously studied.

f) The following substances are now on order for delivery within the next two to three months:

Be_2B, Li_3N, Mg_3N_2, $Li_2O \cdot BeO_2$, $3BeO \cdot B_2O_3$ and $3Al_2O_3 \cdot BeO$.

Additional work on the analysis of literature data will be carried out on substances of interest to the program.

4. HIGH-TEMPERATURE CALORIMETRY

This work includes all enthalpy measurements (heat capacities, heats of fusion, heats of transition, etc.) above approximately room temperature, and uses the "drop" method exclusively. Two apparatuses are available, the first covering the approximate temperature range 300°-1200°K, and the second, the temperature range 1200°-1800°K. The second apparatus is nearly operational, but still awaits tests of the accuracy of measuring the temperature of the sample in the furnace before it can be used routinely with confidence. Because of this fact and also because of the need for data on certain substances at lower temperatures, measurements during the past year were confined to the first apparatus (300°-1200°K), whose accuracy has been well established. Accurate measurements of enthalpy in this temperature range were completed on aluminum carbide (Al_4C_3), beryllium nitride (Be_3N_2), and beryllium aluminate ($BeO \cdot Al_2O_3$). While the samples available were not of the highest purity, their accurate chemical analyses permitted straightforward corrections for the impurities which led to tables of thermodynamic functions given in Appendix B of this report.

With the object of providing high-temperature data on the same substances being measured at low temperatures (see the preceding section 4), future plans are to measure the enthalpies of several substances in the range 300°-1200°K. It is planned to measure during the next fifteen months BeF_2 (crystalline if available, otherwise the glassy form), Li_3AlF_6, Li_2BeF_4, and Be_2C. In addition, a purer sample of $BeO \cdot Al_2O_3$ seems available now, and it is planned to measure this at a few temperatures to compare with the recent results on a less pure but apparently adequate sample.

5. INTERMETALLIC COMPOUNDS OF THE LIGHT ELEMENTS

The literature review of the intermetallic compounds of the light metals has been kept current. Recently the intermetallic compounds of tungsten with aluminum, beryllium, magnesium, and zirconium have been added to the survey.

The synthesis of trimethylhydrazine and tetramethylhydrazine has begun. These materials are desired for heat-of-formation studies.

The research directed toward the preparation of a single, well-defined, crystalline form of beryllium fluoride has begun. At present, the apparatus has been designed and component parts are being procured.

During the coming year the beryllium fluoride research will be vigorously pursued. The problem will be attacked from two directions: (1) the hydrofluorothermal process under pressure, and (2) the phase decomposition of beryllium fluoride under its own vapor pressure.

Detailed analytical work will be carried out on the various hydrides. Preparation and purification work will be carried out as desired by other groups under the program.

Literature searches will be kept current of the alloys and intermetallic compounds.

6. LIGHT-ELEMENT EQUATION OF STATE

The objective of this project continues to be the exploration of the exploding-wire method as a means for producing a two-component system (e.g.vapor of Al or Zr in oxygen) at temperatures between 2000 and 6000°K and pressures up to 100 atmospheres, so that the equation of state of the system under quasi-equilibrium conditions may be determined by experimental measurements. Thus far our effort has concentrated on (1) the study of the hydrodynamic behavior of the exploding-wire system, and (2) the development of experimental techniques of measurement under highly transient conditions.

Activity Summary - July 1, 1961 to June 30, 1962

In the area of instrumentation the development of a large aperture, fast opening shutter for high-speed photography is completed (see last semi-annual report, NBS Report 7437, January 1, 1962). This shutter is capable of opening to an area of 1 x 3 in.^{2} in less than 45 x 10^{-6} sec., with very small attenuation of light intensity. A paper on this work giving construction details and design considerations has been submitted to the NBS Journal of Research, Section C, for publication. Also, an application for a patent on this shutter is being filed by the NBS Patent Committee, following the sponsor's decision against filing.

The calibration work on the measurement of voltage, current and electrical energy under conditions of a high-energy electrical discharge (see semiannual report, NBS Report 7192, July 1, 1962) is being extended to a range of higher voltage, current and frequency. During the past year, our effort has concentrated on (1) the study of the measurement errors, especially those associated with the calorimeter which is used as a reference in energy measurement; and (2) the design and construction of apparatus for the calibration of energy measurement at 120 kv, 400 ka and 750 kc. Some work on the intermediate range (20 kv, 200 ka, and 100 kc) also has been started. The work on density measurement by x-ray absorption did not progress as planned, due to loss of personnel.

In the area of theoretical computation, the detailed numerical method for the first phase of the computation of the flow field behind an expanding cylindrical shock wave has been completed. This computation is needed for the study of the approach to equilibrium of the exploding-wire system. This problem is now being programmed for automatic computation with the aid of a computer. Numerical results are as yet not available.

Plans for Period July 1, 1962 to September 30, 1963

In this period, the work on the calibration of electrical-energy measurement and on the hydrodynamic flow field will be completed. As time and personnel permit, an investigation of simple diatomic molecules, e.g. AlO and ZrO, at high temperatures and pressures will be started.

7. SHOCK WAVE DETERMINATION OF THERMODYNAMIC DATA

A shock-wave investigation of the dissociation kinetics of N_2F_4 was initiated during the past year. The study will be conducted by the measurement of NF_2 concentrations as a function of time by absorption spectrophotometry and of the shock-wave speed. Measurements of density or pressure would provide confirmatory data on the overall thermodynamic state of the shocked gas as deduced from the measured shock-wave speed and the initial state of the gas.

The greater part of the effort was expended in the assembly of the spectroscopic apparatus, and in the modification of the vacuum system and the shock-tube driver section. The existing apparatus, which includes, (a) light screens (wave speed measurements), (b) interferometer (density measurements), and (c) pressure transducer, required little preliminary adjustment.

The NF_2 concentration is determined by observing spectroscopically the change in the optical absorption of $\lambda 2602 (\Delta\lambda = 2A)$ radiation by the shocked gas. The spectroscopic apparatus consists of (a) a UV light source, (b) a grating monochromator (0.5 meter focal length, 16 A/mm. dispersion), (c) photomultiplier detector and oscilloscope recorder, and (d) auxiliary quartz windows and lenses. The light source finally selected is a high-pressure, xenon D.C. arc lamp. It emits a strong continuum which is sufficiently intense and steady in the region of the NF_2 $\lambda 2602$ absorption band. The approximate signal-to-noise ratio and resolving time of this apparatus are, respectively, 80 (theoretical) and 4 microseconds. In a preliminary run with a 2 percent mixture of N_2F_4 in argon (shock Mach number about 1.6), the quartz windows, and particularly the soft glass light screen windows, were etched so severely that the use of sapphire windows was necessitated. The new windows are now on order to the supplier.

The original vacuum system was modified to facilitate the storage and disposal of N_2F_4. A steel gas bottle was included for storage of the experimental gas mixtures at pressures to 10 atmospheres. A soda-lime trap, backed up by a removable cold trap, was inserted to prevent contamination of the pump oil and laboratory by N_2F_4.

The driver section of the shock tube was provided with a mechanical sticker for puncturing the diaphragm after the latter has been loaded to a predetermined pressure. The use of the sticker will accomplish the following: (a) permit the generation of shock waves at closely controlled driver pressures; (b) permit a range of driver pressures (and shock Mach numbers) for a given diaphragm thickness; and (c) facilitate complete opening of the diaphragm, a source of difficulty in previous runs.

A second phase of the activity consists of computations of shock data for the experimental mixtures of N_2F_4 in nitrogen and argon as a function of shock Mach number. The molecular input data for N_2F_4 and NF_2 are those estimated theoretically by Lide on the basis of the harmonic oscillator, rigid rotator approximation. Equilibrium constants used are those determined experimentally by Colburn, et al. These calculations of shock data are still in progress and should be completed soon.

Earlier, while awaiting delivery of the xenon arc lamp, an attempt was made to obtain experimental pressure and density data for comparison with the calculated data. Due to the small differences of pressure and density for the pure diluent gas and the gas mixture, the uncertainty in the experimental data was deemed too great to continue the measurements.

Finally, due to a realignment of the NBS programs, this investigation has been since March, 1961, and will continue to be, under the full sponsorship of this Bureau.

8. HIGH-TEMPERATURE MICROWAVE SPECTROSCOPY

The high-temperature microwave spectrograph was completed during the last year. It has been tested at temperatures up to 700°C with generally satisfactory results. Good spectra were obtained from salts such as thallium chloride which had been previously studied. The microwave transmission of the instrument is rather frequency-sensitive, but in most of the 20,000 - 33,000 mc region sufficient power is available for satisfactory spectroscopy.

Several efforts were made to detect the spectrum of AlCl, but these have so far been unsuccessful. The system used was $Al(l) + AlCl_3(g)$ at a temperature of 650° - 700°C, where calculations predict a significant concentration of AlCl at the usual working pressure of the spectrometer (10^{-3} atmospheres). This system was found to be rather inconvenient because of the difficulty of adjusting the $AlCl_3$ pressure. Consequently, other chemical systems are now being explored as possible sources of AlCl.

If the search for the AlCl spectrum is successful, further experiments on aluminum-halogen systems will be attempted. Some exploratory work will also be done on alkali-metal hydroxides. It appears feasible to detect the spectrum of LiOH. However, because of the very difficult spectroscopic search problem involved with such a light molecule, studies will probably be made first on NaOH or KOH.

9. HALIDE SOLID-VAPOR EQUILIBRIA (TRANSPIRATION METHOD)

The several transpiration measurements on AlF_3 in dry argon which have thus far been completed are in good agreement with values obtained at lower and higher temperatures by other workers. Difficulties with temperature control of the furnace, far greater than anticipated, have greatly slowed the rate of data collection. It has been necessary to study in detail the temperature gradients and vapor diffusion under various conditions of power input, average temperature and control action in order to obtain the best precision during transpiration experiments. Since some of these temperature studies were made while AlF_3 transpiration was being carried out, vapor-pressure values for AlF_3 at four temperatures between 1200° and 1260°K have been obtained. Because of the conditions under which they were obtained, these data are not of the highest precision of which the apparatus is capable. From these data, neglecting dimerization, one obtains, by third-law calculations, an average heat of sublimation $\Delta H^\circ_0 = 70.81 \pm .19$ or $\Delta H^\circ_{298} = 71.26$, which is in very good agreement with presently accepted values. (NBS Report 7192). The uncertainty statement represents the standard deviation from the mean and is probably due in large part to the systematic errors. One serious uncertainty seems to be due to the unknown composition of the AlF_3 sample being used. Attempts to analyze the sample chemically are being hastened.

Future plans call for continuation of the AlF_3 work until the apparatus yields the expected precision. Work on the system AlF_3 + HF and AlF_3 + $AlCl_3$ will then follow.

Background details on this experiment may be found in the following NBS reports:

NBS Report 7192, page 17, July, 1961
NBS Report 6828, page 14, July, 1960
NBS Report 6484, page 4, July, 1959

10. VAPORIZATION OF REFRACTORY SUBSTANCES

The general approach adopted to study experimentally the vaporization of light-metal oxide and other compounds was summarized in the Fourth Technical Summary Report, NBS Report No. 6928, page 12 (July 1, 1960). Some progress in the development of experimental techniques and certain changes of emphasis were further summarized in the Sixth Technical Summary Report, NBS No. 7192, page 20 (July 1, 1961). In a chapter of Part B of the present report a more detailed account of the development, evaluation, and application of the techniques, together with some early results, are presented.

Very briefly, activity during the past year may be summarized as follows: investigation of the BeF_2, BeF_2 - BeO, and BeO systems has commenced and preliminary identification of some of the principal gaseous species have been made in the temperature range 400-2400°C. Further modifications to the apparatus have been started to increase the accuracy of the measurements and to permit the study of the BeF_2 - BeO system under less restricted conditions. Measurements of the rate of vaporization of solid Al_2O_3 using a microbalance technique have been made over the temperature range of about 1850-2150°K. The measurements yielded a useful indication of the probable vaporization coefficient of alumina, but were not of sufficiently high precision to justify further use of the technique at this time. The exploratory study of the application of the arc image furnace in investigations of the vaporization of refractory substances has continued, and preliminary information on the vaporization of liquid alumina in vacuum and in the presence of O_2, H_2, N_2, Ar, and H_2O has been acquired. Some properties of the condensed vapor have also been investigated.

Program Plans July 1, 1962 - October 1, 1963

The following summarizes program plans for the next fifteen months. Broadly speaking all plans are continuations or extensions of presently active or previously discussed experimental investigations of the indicated systems. It is, however, unlikely that all systems will be completely investigated, and unless hampered by experimental difficulties efforts will be concentrated on the higher-priority systems. Plans are listed in order of decreasing priority for the particular experimental techniques.

Mass Spectrometric Technique

1. BeF_2 system — limited mainly by the availability of high purity, crystalline samples.

2. BeO system — using W, Ir, and Re cells. Improvements to the stability of the Knudsen cell supports will be necessary, if the temperature range of the measurements is not to be undesirably restricted.

3. BeF_2 - BeO system — a new cell permitting the condensed fluoride to be kept at a lower temperature than the oxide is under development. If successful, this cell will considerably increase the information that can be gained from this investigation.

Arc Image Technique

1. Al_2O_3 — measurement of rate of free evaporation in a vacuum.

2. Al_2O_3 - O_2, Al_2O_3 - H_2, Al_2O_3 - H_2O — measurement of the rates of vaporization in the presence of various partial pressures of the different gases.

3. Investigation of the possible application of simple mass spectrometric techniques to the study of species vaporizing from Al_2O_3 heated in an arc image furnace.

PART B. THERMODYNAMIC PROPERTIES OF LIGHT-ELEMENT COMPOUNDS

Chapter B-1

THE HEAT OF FORMATION OF ALUMINUM FLUORIDE BY FLUORINE BOMB CALORIMETRY

by Eugene S. Domalski

1. Abstract

The heat of formation of aluminum fluoride has been determined by direct combination of the elements in a bomb calorimeter. The calorimeter was calibrated using standard benzoic acid. In order to attain complete combustion, aluminum powder mixed with finely divided Teflon was burned as a pellet in fluorine at 21 atmospheres pressure. The solid product of combustion was confirmed to be aluminum fluoride by x-ray diffraction analysis. Mass spectrometer analysis showed that the Teflon burned in fluorine to carbon tetrafluoride exclusively. The heat of combustion of the Teflon was determined as 10,352.1 ±0.4 j g^{-1}. The standard heat of formation of aluminum fluoride (ΔHf°_{298}) was found to be -358.3 ±0.3 kcal $mole^{-1}$, based upon the mass of aluminum in the sample.

2. Introduction

The heat of formation of aluminum fluoride was determined under anhydrous conditions by Gross [1,2] and his co-workers, according to the following reaction:

$$(1) \qquad A\ell(c) + \frac{3}{2} PbF_2(c) = A\ell F_3(c) + \frac{3}{2} Pb(c)$$

From a measurement of the heat of reaction, -118.53 ±0.08 kcal $mole^{-1}$, and using -158.5 kcal $mole^{-1}$ for the heat of formation of lead fluoride, they calculated the heat of formation of aluminum fluoride to be -356.3 ±0.3 kcal $mole^{-1}$. In later work, Gross [3] measured the heat of reaction (2) to be -138.31 kcal $mole^{-1}$.

$$(2) \qquad 3NaF(c) + A\ell(c) + \frac{3}{2} PbF_2(c) = Na_3A\ell F_6(c) + \frac{3}{2} Pb(c)$$

Combining this with their heat value for reaction (1), and Coughlin's values [4] for the heat of formation of sodium fluoride and cryolite, they obtained -356.15 kcal $mole^{-1}$ for the heat of formation of aluminum fluoride, independent of the heat of formation of lead fluoride and in excellent agreement with the value they reported earlier.

As a result of 24 experiments, Kolesov, Martinov and Skuratov [5] found a value of -117.7 ± 0.6 kcal mole^{-1} for reaction (1). Using -159.5 kcal mole^{-1} for the heat of formation of lead fluoride, they calculated the heat of formation of aluminum fluoride to be -357 ± 2 kcal mole^{-1}.

A review of the literature for earlier work on the heat of formation of aluminum fluoride reveals the assignment of values ranging from -249.49 to -331.5 kcal mole^{-1} [6-10]. In the final analysis, all these values can be linked to the work of Baud [6,7] who actually measured heats of solution and dehydration of aluminum fluoride hydrates. It was assumed by Baud that without committing a large error the energy of binding of the first molecule of gaseous water in the aluminum fluoride hydrate, $2A\ell F_3 \cdot H_2O$, is the same as that for the first molecule of ammonia in the aluminum chloride ammoniate, $2A\ell C\ell_3 \cdot NH_3$, the value being -33.33 kcal mole^{-1}.

$$2A\ell F_3(c) + H_2O(g) = 2A\ell F_3 \cdot H_2O(c) - 33.33 \text{ kcal.} \tag{3}$$

This assumption or others relating anhydrous aluminum fluoride to its hydrates and its aqueous solution have been used for the calculation of the heat of formation, and their unreliability has affected data for many years. The published estimates of the heat relationships among the anhydrous salt, the hydrates and the aqueous solution, and possibly also Baud's experimental data, may be in error for several reasons.

Aside from Baud's estimate, there are other possible reasons for the lack of agreement in the quoted values for the heat of formation of aluminum fluoride. It has been shown that the rates of attaining equilibrium between aluminum fluoride solutions and the crystalline phases are slow and dependent upon the method by which the hydrates are prepared [11]. The stoichiometry and the varieties of the aluminum fluoride hydrates are not well understood as can be seen by discrepancies in the literature [12,13,14]. Experiments have demonstrated that the heat effects due to the formation of various aluminum fluoride complex ions are significant [15,16].

As the need for confirmatory work on the heat of formation of aluminum fluoride was apparent, the present investigation was undertaken for the purpose of resolving the existing disparity. The direct reaction of aluminum with fluorine was chosen as the method most likely to lead to an unambiguous result. At the time this work was started, investigations by Hubbard, and co-workers [17,18] had demonstrated the feasibility of bomb calorimetry with fluorine as the oxidizer. Those studies however were made on substances forming volatile fluorides, and subsequent publications [19,20,21] have shown the technique to be very successful for that class of compounds. The primary problems expected in undertaking the present study of aluminum were related to the comparatively low volatility of aluminum fluoride. In execution of the experiments the low volatility of the product turned out not to be a major difficulty in comparison with other factors.

3. Preliminary Experiments

Preliminary experiments were made to determine optimum reaction conditions under which aluminum metal would burn in a combustion bomb filled with fluorine. A variety of aluminum samples was tried ranging from pellets to foil to powder. It was found that massive samples, such as pellets or large pieces of foil, would either short out the fuse or fail to burn from the energy put out by the ignited fuse. Aluminum foil cut into narrow shreds (1 in. x 0.010 in. x 0.001 in.) loosely packed together in a combustion bomb, reacted only to about 75 percent completion. Attempts to retain the aluminum shreds as the sample form and improve the degree of completeness of reaction were unsuccessful. From inspection of the inner walls of the bomb after an experiment, and from observations of reactions in a glass combustion vessel, it was evident that shortly after the combustion got underway, burning pieces of aluminum were thrown out of the reaction zone. Upon contact with the cold bomb walls, the reaction was quenched. It was difficult to determine the amount of unburned aluminum because it was intermixed with the combustion product.

Experiments were performed in which aluminum powder contained in a thermoplastic Teflon bag was burned in fluorine. This technique was found undesirable in that only 30 to 50 percent of the aluminum powder reacted. Considerable amounts of carbon were present from incomplete combustion of the Teflon bag.

It was necessary to find a sample geometry and environment which would confine the sample to the reaction zone. Further, it was desirable to have a moderate combustion temperature to avoid burning the sample supports and other bomb parts and still maintain a steady rate of combustion of the sample. It was found that by mixing aluminum powder with finely divided Teflon and pressing the mixture into a pellet, reactions would go essentially to completion (99 to 100 percent). The Teflon made ignition easy because of the low thermal conductivity it imparted to the pellet. In addition it acted as a moderator, kept the sample in the reaction zone, maintained a temperature conducive to burning and prevented bomb parts from substantial attack by fluorine.

4. Materials

The aluminum powder contained the following impurities: silicon, 0.06%; iron, 0.07%; copper, 0.005%; and alumina, 0.47%. The latter was determined by two different methods by the Applied Analytical Chemistry Section. In the first method, aluminum powder was heated in an atmosphere of argon until the powder melted and the oxide floated to the surface. The oxide was then treated by the method of Werner [22] in which the aluminum is dissolved by a bromine-methanol mixture and the Al_2O_3 does not dissolve.

In the second method, a stream of dry argon saturated with bromine is passed over the aluminum in a furnace. The aluminum bromide distills off leaving an aluminum oxide residue behind, which is weighed. The values for $A\ell_2O_3$ content determined by the two methods were 0.46 and 0.47 percent respectively, and the average of all the individual determinations was 0.468 percent.

Inspection of the aluminum powder under a microscope showed a variety of particle sizes ranging from ten microns to 160 microns diameter. The particles were irregularly shaped; the average particle size was determined to be 26 microns by a sub-sieve sizer.

The Teflon powder was composed of irregularly shaped particles, which tended to adhere to one another. Diameters ranged from 50 to 800 microns, as observed by examination under a microscope.

The fluorine gas was analyzed using the mercury absorption technique [23], and found to be 99 percent pure. The residual gases were examined in a mass spectrometer and were shown to be: oxygen, 0.9%; nitrogen, 0.08%; carbon dioxide, 0.01%, with small amounts of silicon tetrafluoride, hydrogen fluoride, fluorocarbons, and other compounds not definitely identified.

5. Preparation of Aluminum-Teflon Samples

About 2.13 grams of Teflon powder was weighed. About 0.40 grams of aluminum powder was added and determined by difference. The powders were then mixed with a needle. The aluminum powder adhered to the Teflon quite readily and thus transfer to a pellet press was not difficult. A loss in weight on pelleting was always observed (1.0 to 2.5 mg.) and it was assumed that the loss of sample took place in proportion to the original amount of each constituent. Buoyancy corrections were applied using 2.702 g cm^{-3} [24] and 2.31 g cm^{-3} [25] for the densities of aluminum and Teflon respectively. The samples were weighed to 0.01 mg.

6. Apparatus

An isothermal-jacket, stirred-water calorimeter was used, which was a modification of the Dickinson design by Prosen and his co-workers [26]. The stirring arrangement was changed to reduce heat transfer from the motors to the jacket. A single motor mounted on an insulated bracket on the jacket wall was used to stir both the jacket and the calorimeter can by a pulley arrangement. The use of this method of stirring, and the operation of the jacket at 30°C made the use of cooling water unnecessary. The jacket water was maintained isothermal with a range of ±0.005°C by a commercial electronic thermoregulator having a temperature sensitive resistor as a sensing element.

Temperatures were measured with a G-2 Mueller Bridge in conjunction with a 25 ohm platinum resistance thermometer. The latter was immersed in the calorimeter near the calorimeter wall. Temperatures were read to 0.0001°C.

Reactions were conducted in a combustion bomb, which is shown in figures 2 and 3 and incorporates features suggested by J. L. Margrave for handling fluorine as the oxidant. The bomb was fabricated from "A" nickel and has a volume of approximately 380 ml.

The standard initial calorimeter for the experiments of Series I was defined as: the combustion bomb with aluminum fuse supports, Chromel C fuse wire, monel pellet holder, 21 atmospheres of fluorine at 303.2°K, the heater, resistance thermometer, calorimeter vessel and a measured quantity of water. The mass of the calorimeter vessel, plus water was 3700.0 grams. For the experiments of Series II, the standard initial calorimeter was the same as for Series I except for the addition of a liner inside the bomb, and slight modifications in the fuse, fuse supports and pellet holder.

The equipment used in measuring the power supplied to the calorimeter during the electrical calibration experiments consisted of the following: Wolff-Dieselhorst potentiometer, 0.01-ohm standard resistor, 20,000 ohm volt box with a ratio of 1000:1, saturated cadmium standard cell, and a 10.6 ohm heater. The current through the heater was controlled by a manual DPDT switch. An electronic timer with a resolution of 10^{-5} sec. was connected to the heater circuit for recording the time during which current flowed through the heater. A standard frequency second signal was used to time the temperature measurements of the calorimeter during the initial and final drift periods of an experiment. Through these periods, temperature readings were taken every minute, while during the main heating period, the time was recorded at integral temperature intervals by a printing-tape chronograph.

The heater used in the calibration experiments was an insulated Advance wire inside a soft copper tube. The tube was flattened and coiled to fit the combustion bomb base.

7. Procedure for Loading and Emptying the Combustion Bomb with Fluorine

A fluorine manifold (figure 1) was used for (1) filling and emptying the combustion bomb, (2) obtaining samples of volatile products of combustion, and (3) obtaining samples of fluorine for analysis.

The manifold consists of a series of packless unions, valves and pressure gages interconnected by means of 1/4 in. monel tubing (wall thickness 0.035 in.). The valves, unions and gages were made of monel or stainless steel and were silver soldered to the monel tubing. In some instances copper couplings were used to facilitate silver soldering a junction. Two special Bourdon gages for fluorine service were used; one in the range 0 to 500 psi, and the other for indicating rough vacuum, 0 to 30 in. Hg. A thermocouple gage was used to measure pressures below 10^{-1} mm Hg. A mechanical pump was found adequate to attain the vacuum needed for working with the fluorine manifold.

The fluorine manifold system was considered to be sufficiently gas-tight for use if no indication of leaks was found at internal pressures of 500 psi and 0.005 mm Hg.

The combustion bomb was attached to the manifold by a screw connector. With valves F, G, M, P, R closed and valves I, K, S and the bomb needle valve open, the bomb was evacuated to 10^{-2} mm Hg. When this vacuum was attained, valves K and S were closed, and fluorine was introduced into the bomb by opening the fluorine tank valve, and then valves D and F. The rate of flow was regulated to allow the pressure to increase about one psi per second. When the pressure on the gage read 300 psi, the bomb needle valve and valve F were closed, then valve D and the fluorine tank valve. If the pressure in the tank is less than 300 psi, it is still possible to fill the bomb to this pressure by the following procedure. A small section of the line, E, is immersed in liquid nitrogen, and fluorine is condensed in it. By allowing the condensed fluorine to evaporate, and regulating the flow through valve D, a pressure of 300 psi can be obtained in the bomb. After the bomb and valve D were closed, the residual fluorine in the manifold was diluted with helium by opening valve G. The mixture was slowly passed through valve P and into the fluorine absorption tower. The absorbent used was soda lime. The rate of flow allowed reduced the pressure about one psi per second. The manifold, including the absorption tower, was filled with helium to 100 psi, and valve Q opened slightly to release the pressure until it was atmospheric. Gases passing through valve Q emerged near the top of the fume hood, in which the apparatus is located, into the path of the up-draft. The purging procedure was performed three times. After closing valve Q, valve R was opened, and the system pumped down through the absorption tower. When about 5 mm absolute pressure had been attained, valve I was closed and the loaded combustion bomb removed from the fluorine manifold.

After an experiment, the bomb was attached to the manifold in order to remove the remaining fluorine, and the procedure was repeated in much the same manner except that the bomb needle valve remained open until the evacuation was complete. The bomb was then filled with one atmosphere of helium and was ready to be opened.

8. Calibration Experiments

Each series of measurements (Series I and II, described later) was accompanied by an electrical calibration in which conditions were the same as in the measurements. Following the experimental measurements on Teflon and the aluminum-Teflon mixtures, two other series of calibration experiments were made.

In Series III benzoic acid (Sample 39h) burned in oxygen was used as a reference material. Also present as part of the bomb conditions were a two cm piece of Chromel C fuse wire supported over the sample with platinum wire leads, a platinum crucible to hold the sample, and one ml of distilled water. The oxygen used was of high purity (99.996%) and no nitric acid titration was required after a combustion experiment. This fact was checked by measuring the pH of the bomb solution after each experiment.

Series IV was an electrical calibration in which the bomb contents and other conditions were the same as the initial conditions of the benzoic acid calibration experiments. The heater was present in both the chemical and electrical calibration experiments.

Because of uncertainties about certain features of the electrical calibration experiments the calibration with benzoic acid, Series III is preferred over Series IV. The ratio of the energy equivalents found in Series III and Series IV was used to correct the energy equivalents of the calorimeters in Series I and II.

Six experiments with benzoic acid in Series III lead to a mean energy equivalent of 143,038.9 ±15.6 j ohm^{-1}. The electrical calibration of Series IV leads to a value of 143,276.5 ±16.0 j ohm^{-1} based on six experiments. For Series I the electrical calibration lead to a value of 143,964.2 ±13.5 j ohm^{-1}, which was corrected by the factor $\frac{143038.9}{143276.5}$ to give 143,725.5 j ohm^{-1}. For Series II the uncorrected and corrected values are 144,337.1 ±14.0 and 144,097.7 j ohm^{-1}, respectively. The uncertainties listed for the energy equivalents are estimates of the standard deviation of the mean.

With the exception of the bomb, the calorimeter was the same for each series of calibration experiments and measurements. The differences in the bomb for the different series are discussed in the section on Apparatus.

9. Combustion Conditions

Series I. An initial series of six electrical calibration experiments, five combustions of Teflon (Table I), and six combustions of aluminum-Teflon mixtures (Table II) were performed. The fuse system used was a 2 cm piece of Chromel C wire (0.006 in. diam.) supported on either side by a 3 cm piece of aluminum wire (0.010 in. diam). The mass of the fuse system, aluminum wires (18 mg) plus Chromel C (3 mg), was 11 mg and its heat of combustion if burned completely was 483.5 j. The mass of the aluminum fluoride formed in these experiments was determined by weighing the bomb head and electrode-fuse system, and the bomb base with the pellet holder before and after each experiment. A balance was used having a capacity of five kg and a readability of 0.5 mg.

Series II. A second series of five electrical calibration experiments, five combustions of Teflon (Table III), and five combustions of aluminum-Teflon mixtures (Table IV) were made. A six cm piece of tungsten wire (0.003 in. diam.) served as the fuse system. The mass of the fuse was about five mg and if burned to completion, contributed 50 j to the combustion. A liner (177 g) was inserted into the bomb base to facilitate the weighing of the aluminum fluoride product. The liner was made of 304 stainless steel (wall thickness 3/32") and fit snugly to the inner dimensions of the bomb (0.003 in clearance). Another monel pellet holder was made to fit inside the liner.

The mass of the aluminum fluoride formed was determined by weighing the stainless steel liner plus monel pellet holder before and after each experiment. Aluminum fluoride deposited on parts of this bomb outside the liner was brushed into the liner for weighing.

Experimental procedures used in the calorimetric measurements have been adequately described elsewhere [27,28].

Atomic weights used in calculating the data were taken from the 1961 Table of Atomic Weights based on Carbon-12, adopted by the International Union of Pure and Applied Chemistry [29]. The unit of energy is the joule and the calorie was was taken as 4.1840 j.

Table I

TEFLON COMBUSTION EXPERIMENTS SERIES I

Experiment No.	Mass Teflon grams	Correction to Energy Equivalent for Fluorine and Teflon joules ohm^{-1}	Corrected Energy Equivalent joules ohm^{-1}	Corrected Temperature Rise ΔR_c ohms	Fuse Energy joules	Standard State Correction joules	Total Energy joules	Heat of Combustion joules gram^{-1}
I-1	4.23389	52.3	143,777.8	0.305338	-153.5	-24.7	43,722.6	10,326.8
I-2	4.24120	52.7	143,778.2	0.305831	-138.5	-24.8	43,808.5	10,329.3
I-3	4.24090	52.6	143,778.1	0.306107	-138.0	-24.8	43,848.7	10,339.5
I-4	4.22823	52.6	143,778.2	0.305673	-349.0	-24.9	43,575.1	10,305.8
I-5	4.24161	53.1	143,778.6	0.306201	- 76.0	-24.9	43,924.3	10,355.6

Average 10,331 joules gram^{-1}

Standard Deviation of Mean ±8

Table II-1

ALUMINUM-TEFLON COMBUSTION EXPERIMENTS SERIES I

Experiment No.	Mass Teflon grams	Mass Aluminum Uncorrected grams	Mass $A\ell F_3$ Recovered, Uncorrected grams	Heat Capacity Correction for Fluorine and Teflon joules ohm^{-1}	Corrected Energy Equivalent joules ohm^{-1}	Corrected Temp. Rise ΔR_c ohms
I-6	2.01775	0.39548	1.2209	30.7	143,756.2	0.299379
I-7	2.13988	0.39914	1.2480	32.1	143,757.6	0.308698
I-8	2.13602	0.40080	1.2510	32.8	143,758.3	0.308887
I-9	2.13445	0.39996	1.2375	30.2	143,755.7	0.309101
I-10	2.13814	0.40224	1.2375	32.2	143,757.7	0.309993
I-11	2.13529	0.40190	1.2625	32.6	143,758.1	0.309959

Table II-2

ALUMINUM-TEFLON COMBUSTION EXPERIMENTS SERIES I

Experiment No.	Fuse Energy joules	Standard State Correction joules	Total Energy joules	Teflon Energy joules	Aluminum Energy, Uncorrected joules	Correction for Metal Impurities and $A\ell_2O_3$ in $A\ell$ grams	Correction for Fluoride Impurities in $A\ell F_3$ grams
I-6	-170.0	-75.2	42,792.4	20,844.8	21,947.6	-0.00239	-0.00366
I-7	-370.0	-76.5	43,931.2	22,107.9	21,823.3	-0.00242	-0.00370
I-8	-195.0	-77.0	44,132.6	22,069.1	22,063.5	-0.00242	-0.00370
I-9	-226.0	-76.2	44.132.8	22,051.8	22,081.0	-0.00242	-0.00370
I-10	-221.5	-77.1	44,265.3	22,089.9	22,175.4	-0.00243	-0.00371
I-11	-308.0	-77.0	44,174.1	22,060.2	22,113.9	-0.00243	-0.00371

Table II-3

ALUMINUM-TEFLON COMBUSTION EXPERIMENTS SERIES I

Experiment No.	Energy Correction for Metal Impurities and $A\ell_2O_3$ joules	$A\ell$ Energy Corrected joules	Moles $A\ell$ in Sample Corrected for Impurities	Moles $A\ell F_3$ Recovered Corrected for Impurities	Heat of Formation based on $A\ell$ kjoules $mole^{-1}$	Heat of Formation based on $A\ell F_3$ kjoules $mole^{-1}$
I-6	-42.8	21,904.1	0.014569	0.014494	1503.53	1511.30
I-7	-43.1	21,780.2	0.014703	0.014817	1481.30	1469.95
I-8	-43.1	22,020.4	0.014765	0.014853	1491.40	1482.56
I-9	-43.1	22,037.9	0.014734	0.014692	1495.74	1499.99
I-10	-43.2	22,132.2	0.014818	0.014817	1493.61	1493.70
I-11	-43.2	22,070.7	0.014805	0.014990	1490.73	1472.36
			Average		1492.7 kj $mole^{-1}$	1488.3 kj $mole^{-1}$
			Standard Deviation of Mean		±3.0	±6.6
			Average		356.8 kcal $mole^{-1}$	355.7 kcal $mole^{-1}$
			Standard Deviation of Mean		±0.7	±1.6

10. Results of Series I Experiments

Of the corrections applied to the heat of combustion of Teflon, and the heat of formation of aluminum fluoride, the fuse energy correction (column 6 of Table I, and column 2 of Table II-2) was by far the largest and most uncertain. The magnitude of this correction was between 0.2 and 0.8 percent of the total energy produced by the combustion process.

Visual observation of the bomb base after a combustion showed many small balls of melted fuse adhering to the wall. Determining the amount of melted fuse remaining was difficult because removal of the fuse from the bomb wall almost invariably resulted in chipping out some of the bomb material itself. Establishing the amount of unburnt fuse through weighing by difference was likewise difficult due to the large mass of the bomb base (2 kg.) and the smallness of the spattered fuse (2 to 6 mg.)

The Teflon energy (column 5, Table II-2) was calculated by multiplying the mass of Teflon used in the aluminum-Teflon pellet by the heat of combustion of Teflon in fluorine, 10,331 j g^{-1}. This latter value was calculated from the combustion of Teflon, alone, in fluorine (Table I).

The aluminum energy uncorrected (column 6, Table II-2), i.e., the energy produced by the combustion of the aluminum and its impurities contained in the aluminum-Teflon pellet, was obtained by subtracting the Teflon energy from the total energy (column 4, Table II-2) released when the mixture was burned in fluorine.

The mass of aluminum fluoride produced in a combustion experiment (column 4, Table II-1) was determined by weighing the bomb base and bomb-head assembly which includes the electrode-fuse system, before and after an experiment. The data reported in column 6 of Table II-3 is the heat of formation of aluminum fluoride based upon the moles of aluminum in the sample prior to the combustion, while the data in column 7 of Table II-3 is the heat of formation of aluminum fluoride based upon the moles of aluminum fluoride found at the end of an experiment.

The following are possible sources of error responsible for the data's dispersion. (1) The degree of fluorination of massive bomb parts such as the bomb head (891 grams) and bomb base (2140 grams) is difficult to establish from differences in mass before and after an experiment. (2) Determining the fraction the fluoride film formed during the combustion period is likewise difficult. It was observed that fluoride films were formed in experiments where no ignition or temperature rise took place. (3) Aluminum fluoride, in a finely divided state, adheres tenaciously to the fluoride film on bomb parts. (4) After a combustion, the flushing procedures necessary to remove the excess fluorine may not only carry small amounts of product into the manifold, but also transport some fluorides on the manifold wall into the bomb.

Table III

TEFLON COMBUSTION EXPERIMENTS SERIES II

Experiment No.	Mass Teflon grams	Correction to Energy Equivalent for Fluorine and Teflon joules ohm^{-1}	Corrected Energy Equivalent joules ohm^{-1}	Corrected Temperature Rise ΔR_c ohms	Fuse Energy joules	Standard State Correction joules	Total Energy joules	Heat of Combustion joules gram^{-1}
II-1	4.25461	55.4	144,153.1	0.306016	-42.7	-25.1	44,045.4	10,352.4
II-2	4.23781	54.7	144,152.4	0.304855	-45.6	-24.8	43,875.2	10,353.3
II-3	4.23486	54.7	144,152.4	0.304558	-42.8	-24.8	43,835.2	10,351.0
II-4	4.22402	54.5	144,152.2	0.303797	-41.8	-24.8	43,726.7	10,351.9
II-5	4.26040	54.9	144,152.6	0.306424	-44.5	-24.9	44,102.4	10,351.7

Average 10,352.1

Standard Deviation of Mean ±0.4 j gram^{-1}

Table IV-1

ALUMINUM-TEFLON COMBUSTION EXPERIMENTS SERIES II

Experiment No.	Mass Teflon grams	Mass Aluminum Uncorrected grams	Mass $A\ell F_3$ Recovered Uncorrected grams	Correction to Energy Equivalent for Fluorine and Teflon joules ohm^{-1}	Corrected Energy Equivalent joules ohm^{-1}	Corrected Temp. Rise ΔR_c ohms
II-6	2.14074	0.40028	1.2311	33.7	144,131.4	0.308652
II-7	2.12728	0.39880	1.2213	34.0	144,131.7	0.306706
II-8	2.14192	0.40031	1.2527	35.2	144,132.9	0.308567
II-9	2.13963	0.40430	1.2661	33.9	144,131.6	0.309709
II-10	2.13579	0.40278	1.2600	33.9	144,131.6	0.308498

Table IV-2

ALUMINUM-TEFLON COMBUSTION EXPERIMENTS SERIES II

Experiment No.	Fuse Energy joules	Standard State Correction joules	Total Energy joules	Teflon Energy joules	Aluminum Energy, Uncorrected joules	Correction for Metal Impurities for $A\ell_2O_3$ in $A\ell$ grams	Correction for Fluoride Impurities in $A\ell F_3$ grams
II-6	-49.2	-76.9	44,360.3	22,161.2	22,199.1	-0.00242	-0.00370
II-7	-49.6	-76.7	44,079.8	22,021.8	22,058.0	-0.00241	-0.00368
II-8	-50.1	-77.3	44,347.3	22,173.4	22,173.9	-0.00242	-0.00370
II-9	-50.2	-78.5	44,511.1	22,149.7	22,361.4	-0.00245	-0.00373
II-10	-49.8	-77.2	44,337.3	22,109.9	22,227.4	-0.00244	-0.00371

Table IV-3

ALUMINUM-TEFLON COMBUSTION EXPERIMENTS SERIES II

Experiment No.	Energy Correction for Metal Impurities and $A\ell_2O_3$ joules	$A\ell$ Energy Corrected joules	Moles $A\ell$ in Sample, Corrected	Moles $A\ell F_3$ Recovered, Corrected	Heat of Formation based on $A\ell$ kjoules mole^{-1}	Heat of Formation based on $A\ell F_3$ kjoules mole^{-1}
II-6	-43.1	22,156.0	0.014746	0.014616	1502.51	1515.87
II-7	-43.0	22,015.0	0.014691	0.014499	1498.54	1518.38
II-8	-43.1	22,130.8	0.014747	0.014873	1500.70	1487.98
II-9	-43.4	22,318.0	0.014894	0.015033	1498.46	1484.60
II-10	-43.2	22,184.2	0.014838	0.014960	1495.09	1482.90
			Average		1499.1 kj mole^{-1}	1498.0 kj mole^{-1}
			Standard Deviation of Mean		±1.2	±7.9
			Average		358.3 kcal mole^{-1}	358.0 kcal mole^{-1}
			Standard Deviation of Mean		±0.3	±1.9

11. Results of Series II Experiments

The estimation of the energy contributed by the fuse system was apparently improved by replacing the aluminum-Chromel C fuse by tungsten, as can be seen from the greater precision of the measurements based on the aluminum in the sample. This may be demonstrated by comparing the fuse energy corrections of Series I (column 2, Table II-2) with those of Series II (column 2, Table IV-2). In Series II, the fuse energy correction is about 0.1 percent of the total energy for the combustion process. The absence of large amounts of spattered fuse implies a more thorough fuse combustion.

The aluminum fluoride produced from buring aluminum was collected in the stainless steel liner. Any aluminum fluoride powder adhering to the bomb head assembly or present in the space between the liner and bomb base was brushed into the liner and weighed.

The data reported in column 6, Table IV-3, is the heat of formation of aluminum fluoride based upon the moles of aluminum in the sample prior to combustion, while the data in column 7, Table IV-3, is the heat of formation of aluminum fluoride based upon the moles of aluminum fluoride weighed found at the end of an experiment. Use of the liner gave poorer precision to the calculated value for the heat of formation of aluminum fluoride based upon the $A\ell F_3$ recovered. The following reasons might offer an explanation for these findings: (1) The liner has a large surface area of metal exposed for fluoride film formation than did the bomb head and bomb base combined. (2) Quantitative transfer of small amounts of fluoride product from bomb parts is a difficult task.

12. Discussion

The aluminum fluoride produced in combustions was examined microscopically and found to be crystalline in appearance. All particles were regularly shaped and had diameters of three to five microns. X-ray diffraction analyses of aluminum fluoride agreed well with the data reported earlier [30]. The samples had the space group D_3^7 - R32 #155 which is trigonal with a hexagonal cell, a = 4.927A and c = 12.445 A, and six molecules per unit cell.

Mass spectrometric analyses of the products of combustion formed when Teflon burns in fluorine showed carbon tetrafluoride to be the only product.

After a Teflon combustion, a small amount of carbon residue was discernible (0.2 to 0.9 mg). No correction was applied since it was assumed that the carbon formation took place during an aluminum-Teflon combustion in an amount proportional to the mass of the Teflon present. Thus, the error due to carbon formation would cancel out when the Teflon energy was subtracted from the total energy released from the combustion process.

Data on the surface energy of aluminum fluoride is not available, however, a crude extrapolation can be made from work done on alkali halides [31,32]. Using four microns as the particle diameter of the aluminum fluoride formed in the combustion process, 3.197 g cm^{-3} as the density [30], and assuming a surface energy of 2 x 10^3 erg cm^{-2}, one finds the energy contribution to be less than 0.005%.

An experiment was performed in a glass combustion vessel where aluminum burned in a 50-50 mixture of fluorine and oxygen. The white powder formed as a result of the combustion was analyzed by x-ray methods and found to be solely aluminum fluoride and not a mixture of aluminum fluoride and alumina. Because of these findings, no correction has been applied for the oxygen impurity in the fluorine.

Of the heat of formation values calculated for aluminum fluoride, the most reliable is that of Series II, 358.3 ±0.3 kcal $mole^{-1}$, which is based on the amount of aluminum present in the sample. The large errors introduced because of the fuse energy correction in Series I, and the difficulty in collecting and weighing the aluminum fluoride formed as a product of combustion precludes the choice of the heat of formation based on this data.

The present work is in reasonably good agreement with other recent investigations on the heat of formation of aluminum fluoride [1,2,5]. The work of Gross laid the basis for suspecting the validity of the previously determined heat values based on solution calorimetry. The later work of Gross [3] and the studies of Kolesov, Martinov and Skuratov clearly indicated the heat of formation of aluminum fluoride was in the range 355 to 359 kcal $mole^{-1}$. However, the study of the reaction of aluminum with lead fluoride has several disadvantages. Because of analytical problems the products of combustion were not separated and determined individually, but the completeness of the reaction was suggested by the consistency of the data. The mode of preparing lead fluoride has an apparent effect upon the heat of reaction. Ascertaining whether the heat of reaction was influenced by the high temperature interaction of lead with aluminum is not easily resolved. Finally, although the reaction of lead fluoride and aluminum can lead to a heat of formation value for aluminum fluoride, provided the heat of formation of lead fluoride is known, it is not a direct determination.

The present work has considered areas previously neglected. The products of combustion of the reaction of an aluminum-Teflon sample have been positively identified, and the mass of aluminum fluoride recovered after a combustion experiment has been determined. The oxide content of aluminum powder was shown to be significant and a correction applied for its presence.

13. Calculation of Fuse Energy

Series I. Aluminum-Chromel C fuse system.

The energy evolved per unit mass by the combustion of Chromel C in fluorine was calculated from the heats of formation of the fluorides in the alloy [10]. Each miligram of Chromel C burned in fluorine produces 14.5 joules.

Assuming the heat of formation of aluminum fluoride to be -356 kcal mole^{-1}, 55 joules are produced per milligram of aluminum burned in fluorine.

$$
\begin{aligned}
(55 \text{ joules})\ (8 \text{ mg}) &= 440 \\
(14.5 \text{ joules})(3 \text{ mg}) &= \underline{\ 43.5} \\
&\ 483.5 \text{ joules/11 mg fuse system.}
\end{aligned}
$$

Series II. Tungsten Fuse Wire.

The heat of formation of $WF_6(g)$ is -416 kcal mole^{-1} [33]. The combustion of 5.25 mg of tungsten wire gives off 50 joules.

14. Constants used in Calculation of Data

The standard state corrections were modified in order to account for the use of fluorine as the oxidant [34]. The coefficient $[\frac{\partial E}{\partial P}]_T$ required to reduce ΔE bomb conditions to ΔE standard state conditions was estimated from the force constants for fluorine [35] and carbon tetrafluoride [36]. The heat capacity at constant volume [37] for fluorine used was 5.52 cal deg^{-1} mole^{-1}. Heat capacities at constant pressure of 0.217, 0.28, 0.215, and 0.1674 cal. deg^{-1} gram^{-1} for aluminum [38], Teflon [39], aluminum fluoride [40] and carbon tetrafluoride [41].

It was assumed that the metallic impurities and the alumina reacted completely with fluorine. Mass and energy corrections were applied using -235, -372.4, and -126.9 kcal mole^{-1} for the heats of formation of ferric fluoride, silicon tetrafluoride, and cupric fluoride [10], respectively.

15. Conclusion

(1) The heat of formation of aluminum fluoride has been determined by direct combination of the elements in a bomb calorimeter.

$$A\ell(c) + \frac{3}{2} F_2(g) = A\ell F_3(c), \quad \Delta H^o_{f298.15} = 358.3 \pm 0.3 \text{ kcal mole}^{-1}$$

This value is based upon the mass of aluminum in the sample.

(2) By mixing aluminum powder with finely divided Teflon, complete combustion of the metal was found possible. The application of powdered Teflon to other metal powders for combustion reactions is apparent.

(3) Determining the mass of aluminum fluoride formed in a combustion experiment has met with moderate success, however, further work will be needed in order to improve the precision of the method.

(4) The low energy contribution of a tungsten fuse per unit mass shows it to be superior to the aluminum-Chromel C fuse in fluorine bomb combustions.

16. Bibliography

1. P. Gross, C. Hayman, and D. L. Levi, Trans. Faraday Soc. 50, 477-80 (1954).
2. P. Gross, C. Hayman, and D. L. Levi, "Bull. of Chem. Thermodynamics", No. 2, 21 (1959).
3. P. Gross, C. Hayman, and D. L. Levi, "International Symposium on Physical Chemistry in Process Metallurgy", Pittsburgh, April 1959.
4. J. P. Coughlin, J. Am. Chem. Soc. 80, 1802 (1958).
5. V. P. Kolesov, A. M. Martinov, and S. M. Skuratov, Zhur. Neorg. Khim. 6, 2623 (1961).
6. E. Baud, Compt. rend. 135, 1105 (1902).
7. E. Baud, Ann. chim. phys. 1, 8 (1904).
8. H. von Wartenberg, Z. anorg. Chem. 151, 329 (1926).
9. F. R. Bichowsky and F. D. Rossini, "The Thermochemistry of Chemical Substances", Reinhold Publishing Co., New York, 1936.
10. F. D. Rossini et al., "Selected Values of Chemical Thermodynamic Properties", NBS Circular 500, February 1952.
11. W. F. Ehret and F. J. Frere, J. Am. Chem. Soc. 67, 64-68 (1945).
12. H. J. Emeleus, Chapter I, "Fluorine Chemistry", J. H. Simons, Editor, Vol. I, Academic Press, Inc., New York, 1950, p. 40.
13. A. Seidell and F. W. Linke, "Solubilities, Inorganic and Metal Organic Compounds", 4th Edition, Vol. I, D. Van Nostrand Co. Inc., Princeton, 1958, p. 178-9.

14. I. G. Ryss, Khimiya ftora i ego neorganicheskikh soedinenii (Gosudarstvennoe Nauchno-Technicheskse Izdatel'stvo Khimicheskoi Literatury, Moskva, 1956.) Available in English as: "The Chemistry of Fluorine and its Inorganic Compounds" (Translated from a publication of the State Publishing House for Scientific, Technical and Chemical Literature, Moscow, 1956, F. Haimson, translator) AEC-tr-3927 (Parts 1 and 2) (Office of Technical Services, Department of Commerce, Washington 25, D. C., 1960).

15. W. M. Latimer and W. L. Jolly, J. Am. Chem. Soc. 75, 1548 (1953).

16. E. L. King and P. K. Gallagher, J. Phys. Chem. 63, 1073 (1959).

17. W. N. Hubbard, Bull. Chem. Thermodynamics, No. 3, 2 (1960).

18. W. N. Hubbard, J. L. Settle, and H. M. Feder, Proc. Symp. Thermodynamics, Fritzens-Wattens, Austria, Aug. 1959. Pure Appl. Chem. 2, 39-44 (1961).

19. E. Greenberg, J. L. Settle, H. M. Feder, and W. N. Hubbard, J. Phys. Chem. 65, 1168-72 (1961).

20. J. L. Settle, H. M. Feder, and W. N. Hubbard, J. Phys. Chem. 65, 1337-40 (1961).

21. S. S. Wise, J. L. Margrave, H. M. Feder, and W. N. Hubbard, J. Phys. Chem. 65, 2157-9 (1961).

22. O. Werner, Metall. 4, 9-12 (1950).

23. G. T. Armstrong and R. S. Jessup, J. Research Natl. Bur. Standards 64A, 49 (1960).

24. J. D. Edwards and T. A. Moormann, Chem. and Met. Eng. 24, 61-4 (1921).

25. Density determined experimentally.

26. E. J. Prosen, W. H. Johnson and F. Y. Pergiel, J. Research Natl. Bur. Standards 62, 43-47 (1959).

27. F. D. Rossini, "Experimental Thermochemistry", Chapters 3 and 6, Interscience Publishers, Inc., New York, 1956.

28. R. S. Jessup, NBS Monograph 7, "Precise Measurement of Heat of Combustion with a Bomb Calorimeter", February 26, 1960.

29. Chem. Eng. News, 38, page 43, November 20, 1961.

30. E. Staritzky and L. B. Asprey, Anal. Chem. 29, 984 (1957).

31. G. C. Benson, P. Balk, and P. White, J. Chem. Phys. <u>31</u>, 109 (1959).

32. G. C. Benson, E. Dempsey, and P. Balk, J. Chem. Phys. <u>34</u>, 157 (1961).

33. O. E. Myers and A. P. Brady, J. Phys. Chem. <u>64</u>, 591 (1960).

34. W. N. Hubbard, Chapter 5, Vol. II, "Experimental Thermochemistry", H. A. Skinner, Editor, Interscience Publishers, Inc., New York, N.Y., pages 95-127.

35. D. White, J. H. Hu, and H. L. Johnston, J. Chem. Phys. <u>21</u>, 1149 (1953).

36. D. R. Douslin, Thermodynamics Laboratory, Contribution No. 109, U.S. Bureau of Mines, Bartlesville, Oklahoma.

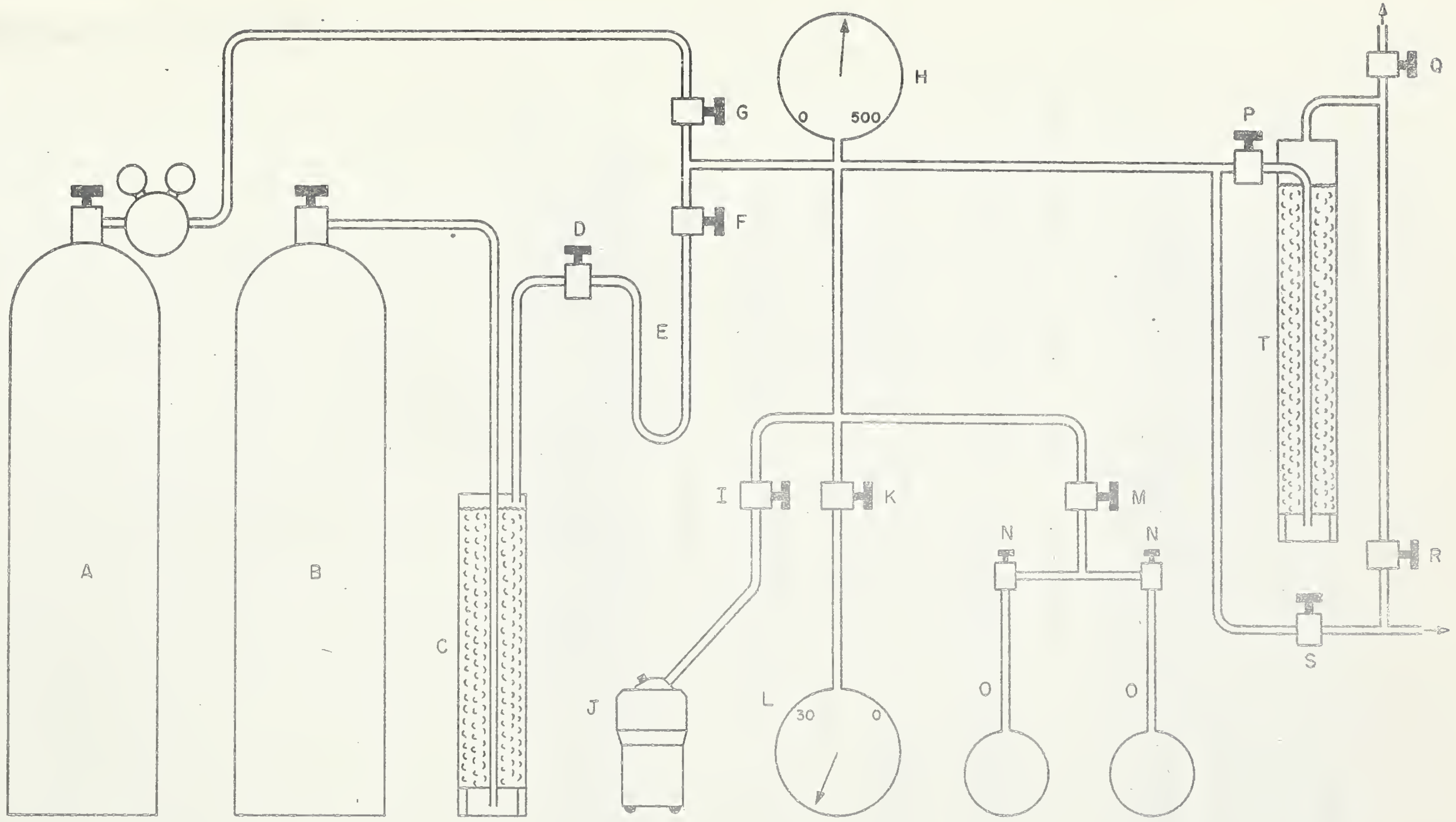
37. W. H. Evans, T. R. Munson, and D. D. Wagman, J. Research Natl. Bur. Standards <u>55</u>, 147 (1955).

38. W. F. Giauque and P. F. Meads, J. Am. Chem. Soc. <u>63</u>, 1897 (1941).

39. W. D. Good, D. W. Scott, and G. Waddington, J. Phys. Chem. <u>60</u>, 1080 (1956).

40. J. O'Brien and K. K. Kelley, J. Am. Chem. Soc. <u>79</u>, 5616 (1957).

41. K. K. Kelley, "Contributions to the data on theoretical metallurgy, XIII. High temperature heat-content, heat-capacity, and entropy data for the elements and inorganic compounds", U. S. Bureau of Mines Bull. 584, U. S. Government Printing Office, Washington 25, D.C., 1960.



A. HELIUM
B. FLUORINE
C. HYDROGEN FLUORIDE TRAP
D. FLUORINE VALVE
E. LIQUID NITROGEN TRAP FOR FLUORINE
F. FLUORINE VALVE TO MANIFOLD
G. HELIUM VALVE TO MANIFOLD

H. PRESSURE GAUGE (0-500 P.S.I.)
I. BOMB VALVE
J. BOMB
K. VACUUM GAUGE VALVE
L. VACUUM GAUGE (0-30 IN. Hg)
M,N. GAS SAMPLE COLLECTOR VALVES
O. GAS SAMPLE COLLECTOR BULBS

P. FLUORINE ABSORPTION TOWER VALVE
Q. VENT VALVE TO EXHAUST HOOD
R. VACUUM VALVE VIA FLUORINE ABSORPTION TOWER.
S. DIRECT VACUUM VALVE
T. FLUORINE ABSORPTION TOWER

FIG. I. SCHEMATIC DIAGRAM OF FLUORINE MANIFOLD

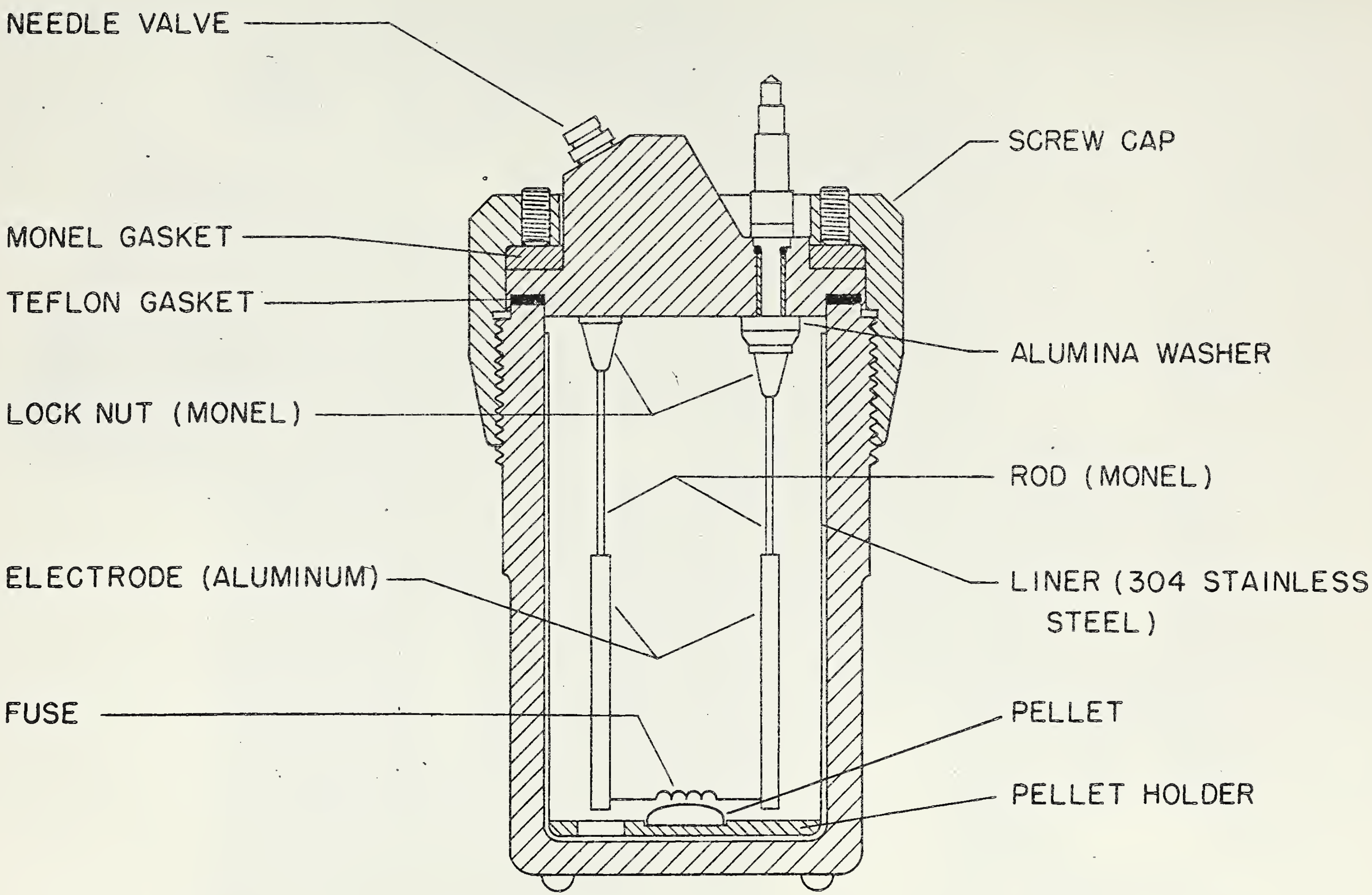


FIG. 2. INNER BOMB ARRANGEMENT

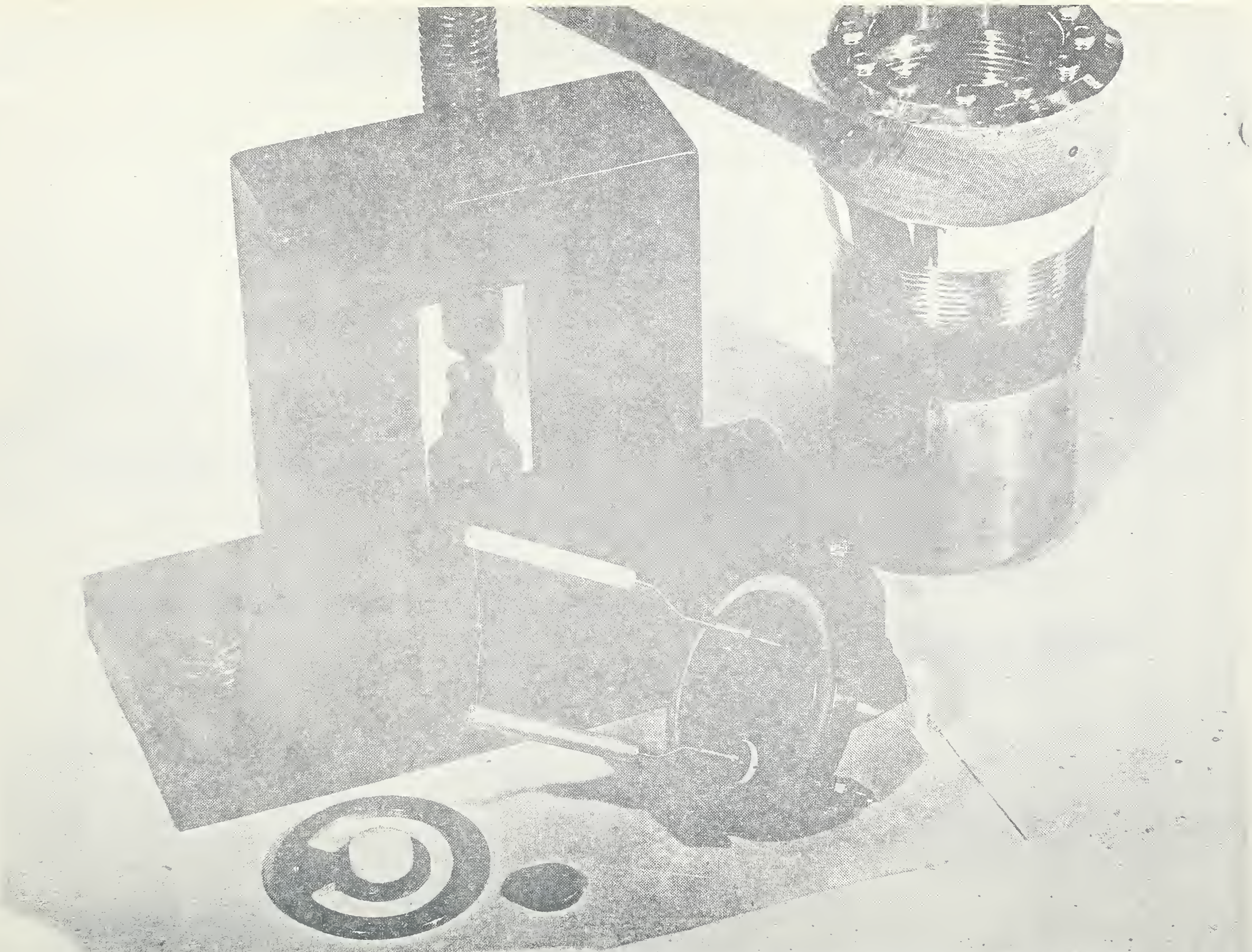


FIGURE 3. PELLET PRESS, PELLETS, ELECTRODE SYSTEM

Chapter B-2

ALUMINUM CARBIDE. MEASUREMENTS OF THE LOW-TEMPERATURE HEAT CAPACITY AND CORRELATION OF THE RESULTS WITH HIGH-TEMPERATURE ENTHALPY DATA

by William G. Saba and George T. Furukawa

No low-temperature heat-capacity data on aluminum carbide, $A\ell_4C_3$, have been reported in the literature. Estimates of S^o_{298} have, however, been given in a number of compilations [1,2,3,4,9]. The value S^o_{298} = 25.0 ±3 e.u., not in disagreement with the above estimates, was listed in NBS Report 6645 [6]. In NBS Report 7437 [11] were described results of the recent relative enthalpy measurements obtained at the National Bureau of Standards in the range 273° to 1173°K. A table of thermodynamic functions for $A\ell_4C_3$ was calculated and given in NBS Report 7437 [11] (Table B-59) based on the results of these heat measurements and on the above estimated value of S^o_{298} = 25.0 ±3 e.u. The results of the low-temperature heat-capacity measurements, to be described subsequently in this chapter, will show that S^o_{298} is significantly lower than the estimated value. A revised table of thermodynamic functions (Table B-59 Revised, Appendix B) has been calculated based on these new measurements, as well as on the above NBS enthalpy measurements from 273° to 1173°K.

The aluminum carbide sample used in the low-temperature heat-capacity measurements was taken from a larger sample supplied by the Aluminum Company of America, ALCOA Research Laboratories. The samples (specimens) used in the high-temperature measurements were taken also from this larger sample. The sample was analyzed by R. A. Paulson of the Applied Analytical Research Section at the Bureau both before and after the heat-capacity measurements. The results of these chemical analyses are given in Table 1. The first analysis did not include a determination for iron. The agreement between analyses is relatively good considering both the uncertainties in the analytical methods and possible small inhomogeneities in the sample. The analysis on the portion of $A\ell_4C_3$ sample after the heat-capacity measurements were made was used as the basis for correcting the sample for impurities. The percentages were normalized so as to give a total of 100 percent, as shown in Table 1.

Table 1

Chemical Analysis of $A\ell_4C_3$

COMPONENT	PORTION OF SAMPLE BEFORE MEASUREMENTS Percentage by weight	PORTION OF SAMPLE AFTER MEASUREMENTS Percentage by weight	NORMALIZED PERCENTAGES
Aluminum Carbide	94.8	94.8	94.46
Free Aluminum	1.3	1.0	1.00
Free Carbon	0.7	1.0	1.00
Aluminum nitride	1.3	1.3	1.29
Aluminum oxide	2.0	2.2	2.19
Iron	not determined	0.06	0.06
TOTAL	100.1	100.36	100.00

The sample was loaded into the container in a controlled-atmosphere box using argon gas (dew-point of -50°C). At the same time, portions of the sample were sealed in test tubes under dry argon gas for chemical analysis. The container plus the sample was evacuated and purged with helium gas several times. Helium gas at a pressure of 5.8 cm Hg was sealed in the container with the sample.

A total of 109 heat-capacity determinations were made over the range 18° to 390°K.

After the heat measurements the sample was removed from the container in the controlled-atmosphere box using again argon gas (dew-point -50°C). The removed sample was sealed in test tubes under dry argon for chemical analysis. Heat-capacity measurements were then made on the empty container over the same temperature range mentioned above, in a total of 87 determinations.

The experimental data were fitted to empirical equations over selected, overlapping temperature intervals by the method of least squares using a digital computer code. These overlapping equations were joined together at temperatures of the most favorable combinations of values of the heat capacity and its first and second derivatives. The resultant series of heat capacities at integral temperatures obtained from the above process was smoothed by a 9-point cubic smoothing code on the computer. The net values of the heat capacity, obtained by differencing the smoothed gross and empty values at the corresponding temperatures, were corrected for the impurities and helium exchange gas and again checked for smoothness. A Debye heat-capacity function, fitted to the smoothed values at the lower temperatures, was used to obtain the values from 0° to 15°K. The resultant net, smoothed heat capacities were integrated using four-point Lagrangian integration coefficients and the various thermodynamic functions evaluated up to 390°K.

The high-temperature relative enthalpy data of Victor, Thurber and Douglas [11] were refitted, by the method of least squares, to equations of the type:

$$C_p = A + BT + \cdots + D/T + E/T^2 + \cdots$$

The equation which best fit the data was:

$$C_p = 47.556 + 3.85 \times 10^{-4}\ T - 5.842 \times 10^3/T$$

The smoothed low-temperature data were merged into the high-temperature data calculated from the above equation over the range 270° to 380°K such that the resultant enthalpy change from 273.15° to 373.15°K was about the average of the value from the low-temperature data and that from the high-temperature relative-enthalpy measurements. The final enthalpy change calculated for the temperature interval was 2936 cal/mole as compared with 2933 cal/mole obtained in the low-temperature measurements and with 2939 cal/mole obtained in the high-temperature measurements.

Since the relative-enthalpy data ended at approximately 1200°K, an attempt was made to extrapolate an appropriate equation above 1200°K to 2000°K on the basis of entropy calculated from high-temperature vapor-pressure data.

The most recent vapor-pressure data is that of Meschi and Searcy [5] on the dissociation pressure of Al_4C_3. Treatment of their data yielded an entropy for Al_4C_3 at 1800°K of 96 ±6 e.u. The uncertainty of ±6 e.u. is based on an uncertainty of ±10 kcal/mole of Al_4C_3 in the $\Delta H°$ given by Meschi and Searcy. Analysis of the work of Prescott and Hincke [8] on the equilibria of the Al_4C_3 - N_2 system yielded a value of 94 e.u. for the entropy of Al_4C_3. Although this agrees fairly well with the result based on the data of Meschi and Searcy [5], it does not agree with the value calculated from some earlier data of Prescott and Hincke [7] on the Al_2O_3 - C system, which yielded 64 e.u. for the entropy of Al_4C_3 at 1800°K. There is, however, considerable uncertainty as to the nature of the reactants and products involved in the Al_2O_3 - C system. In still poorer agreement is the value of 111 e.u. for the entropy of Al_4C_3 at 1800°K calculated from the approximate vapor pressures obtained from the work of Ruff [10]. The disagreement is readily understood when one considers that an error in the pressure of a factor of two results in a change of approximately 6 e.u. for the entropy of formation at 1800°K.

The high-temperature relative enthalpy data could not be reasonably extrapolated above 1200°K to the entropies calculated from the vapor-pressure data, for even the most favorable value of 94 e.u. for the entropy of Al_4C_3 at 1800°K (based on Prescott and Hincke [8]) would require the heat capacity to be unreasonably high at 1800°K (approximately 70 cal/deg mole).

It was decided to extrapolate the data on the basis of the above equation which best fit the relative-enthalpy data of Victor, Thurber and Douglas [11], as this equation was of an acceptable form for high-temperature heat capacities and was well behaved in terms of heat capacity and its derivatives up to 2000°K.

The various thermodynamic functions were evaluated from the final accepted values of heat capacity from 0° to 2000°K. The results are given in Table B-59 (Appendix B) along with the final smoothed heat capacities. The experimental value of S°_{298} was found to be 21.3 e.u. as compared to the estimated value of 25 e.u. The value of $S^\circ_{1800} = 91$ e.u. is well within the uncertainty of the vapor-equilibria data. Table B-59 revised in Appendix B of the present report supersedes Table B-59 of NBS Report 7437 and Table B-37 of NBS Report 6928.

References

1. L. Brewer, L. A. Bromley, P. W. Gilles and N. L. Lofgren, Thermodynamic and Physical Properties of Nitrides, Carbides, Sulfides, Silicides, and Phosphides, Paper No. 4; Chemistry and Metallurgy of Miscellaneous Materials: Thermodynamics, National Nuclear Energy Series Vol. 19B, edited by L. L. Quill, McGraw-Hill Book Company, Inc., New York, 1950.

2. K. K. Kelley, Contributions to the Data on Theoretical Metallurgy. VIII. The Thermodynamic Properties of Metal Carbides and Nitrides, Bureau of Mines Bulletin 407, 1937.

3. O. H. Krikorian, High Temperature Studies; Part II, Thermodynamic Properties of the Carbides, UCRL 2888, April, 1955.

4. O. Kubaschewski and E. Ll. Evans, Metallurgical Thermochemistry (Pergamon Press, Ltd., London, 1958, Third Edition) (Also earlier editions).

5. D. J. Meschi and A. W. Searcy, "The Dissociation Pressure of Aluminum Carbide," J. Phys. Chem. 63, 1175-1178 (1959).

6. "Preliminary Report on the Thermodynamic Properties of Selected Light-Element Compounds", NBS Report 6645, National Bureau of Standards, Washington, D.C., 1 January 1960 (Amended 1 April 1960), pp. 12 and 16.

7. C. H. Prescott, Jr. and W. B. Hincke, "The High-Temperature Equilibrium Between Aluminum Oxide and Carbon", J. Am. Chem. Soc. 49, 2753-2759 (1927).

8. C. H. Prescott, Jr. and W. B. Hincke, "Equilibrium Between Aluminum Carbide and Nitrogen at High Temperatures", J. Am. Chem. Soc. 50, 3228-3237 (1928).

9. F. D. Rossini, D. D. Wagman, W. H. Evans, S. Levine and I. Jaffe, Selected Values of Chemical Thermodynamic Properties, National Bureau of Standards Circular 500, February, 1952.

10. O. Ruff, E. Jellinek and T. Foehr, "Constitution and Thermal Stabilities of Carbides", Z. Elektrochem. 24, 157-62 (1918).

11. A. C. Victor, W. R. Thurber and T. B. Douglas, "Aluminum Carbide: High-Temperature Thermodynamic Functions Based on Recent Measurements of Heat Capacity at the National Bureau of Standards", Preliminary Report on the Thermodynamic Properties of Selected Light-Element and Some Related Compounds, NBS Report 7437, National Bureau of Standards, Washington, D. C., 1 January 1962, pp. 13-18.

Chapter B-3

Be_3N_2 AND $BeO \cdot Al_2O_3$: HIGH-TEMPERATURE THERMODYNAMIC FUNCTIONS BASED ON RECENT MEASUREMENTS OF HEAT CAPACITY AT THE NATIONAL BUREAU OF STANDARDS

by Thomas B. Douglas and William H. Payne

Samples: Sources and Compositions

(a) Be_3N_2: The sample was obtained from the Brush Beryllium Company, of Cleveland, Ohio, who produced it by heating pure beryllium metal in nitrogen and crushing the product to a particle size of from -20 to +50 mesh. The supplier agreed to specifications of a minimum content (by weight) of 97.0% Be_3N_2 and a maximum content of 2.0% BeO, 0.75% Be metal, 0.08% C, 0.08% Aℓ, 0.015% Cr, 0.08% Fe, and 0.01% Mn. Quantitative chemical analyses for total Be and total N were performed by Rolf A. Paulson, of the Applied Analytical Research Section of the Bureau, by weighing the Be as BeO and distilling off the N as NH_3. These analyses conformed closely to the suppliers' specification limits stated above in the case of the original sample, but indicated 48.14 ±0.08% total N (3 analyses) and 48.65 ±0.02% total Be (2 analyses) in the case of the sample on which the heat-capacity measurements had been made (indicating some hydrolysis during handling). (The amounts of F and Cℓ found were approximately 0.0005 and 0.01% respectively.) Since a spectrochemical analysis for the minor constituents is not yet available, it was assumed that the sample thermally measured contained C, Aℓ, Cr, Fe, and Mn (the metal oxides weighed as BeO) in the amounts shown in Table 1 and that the remainder was entirely Be_3N_2, BeO, and Be metal. The above analyses then determined the percentages of the last three substances stated in the table.

(b) $BeO \cdot Al_2O_3$: The sample used was prepared by Stephen Hasko, of the NBS Engineering Ceramics Section, by mixing (without use of a "binder") the stoichiometric amounts of powdered BeO and Al_2O_3 (both 99.9% or purer), heating for one hour at 1775°C, regrinding and repressing into pellets, and then heating for two hours at 1800°C. (According to the analyses of the product stated in Table 1, a small part of the BeO volatilized during the heating.)

A considerable amount of work has been reported on elucidating the system $BeO–Al_2O_3$, including the detailed study by Lang, Fillmore and Maxwell [1]. They verified the existence of two congruent-melting compounds, $BeO \cdot Al_2O_3$ (which occurs naturally in impure form as the mineral chrysoberyl) and $BeO \cdot 3Al_2O_3$, whose melting points they found to be 1870° ±10°C and 1910° ±10°C respectively. They found a more than

95% conversion to $BeO \cdot Al_2O_3$ by heating an equimolar mixture of the two component oxides at 1250°C for four hours. (The two oxides in this system have so nearly the same optical properties that they cannot be distinguished from each other by optical means.)

The sample of $BeO \cdot Al_2O_3$ used in the present work was examined petrographically (microscopically) by Alvin Van Valkenburg, of the NBS Constitution and Microstructure Section. He found the particle size to be generally greater than 50 microns. He observed the material to have an index of refraction concordant with that reported for this compound except for an estimated 20% of the volume composed of cavities which were thought to be voids but could conceivably have been regions of the unreacted oxides BeO and Al_2O_3.

The sample was examined also by H. Steffen Peiser, of the NBS Crystal Chemistry Section, who determined an X-ray-diffraction pattern of it. Several strong lines were found characteristic of the crystal $BeO \cdot Al_2O_3$, but there was no evidence by this method of examination of any lines known to be associated with either BeO or $BeO \cdot 3Al_2O_3$ as separate crystalline phases. The diffraction pattern gave evidence of a small amount of crystalline Al_2O_3 (a finding which is consistent with the small excess of this oxide, over the stoichiometric percentage in $BeO \cdot Al_2O_3$, as found in the chemical analysis described below). In addition, there were several lines (not found for a somewhat purer sample of $BeO \cdot Al_2O_3$ examined simultaneously) which indicated a small amount of one or more foreign crystalline phases; since no suitable standards were available, however, this impurity could not be identified nor its amount estimated from the X-ray results.

The $BeO \cdot Al_2O_3$ sample was analyzed chemically for Al and Be by Thomas J. Murphy, of the NBS Applied Analytical Research Section. After crushing and subsequent leaching to remove all Fe picked up from the mortar, the sample was completely dissolved in concentrated HCl during 24 hrs. at 250°-300°C. (The small insoluble residue proved to be almost entirely SiO_2.) At pH 4.2-4.5, 8-hydroxyquinoline (in acetic acid) precipitated the Al, which was fired and weighed as Al_2O_3. At pH 8-9, the Be was then precipitated as $Be(OH)_2$ and finally weighed as BeO. Control tests of the method on known mixtures of BeO and Al_2O_3 gave excellent results. The sample of $BeO \cdot Al_2O_3$ was found to contain, by weight, 80.88 ±0.03% Al_2O_3 (2 analyses) and 19.05 ±0.05% BeO (3 analyses), corresponding to a mole ratio Al_2O_3/BeO of 1.041. Pending a spectrochemical analysis not yet available, the percentages given in Table 1 have been normalized to total 100%. These analyses, of course, give no information on how much of the Al_2O_3 and BeO are combined in one or both of the two compound oxides.

Table 1

Assumed Stoichiometric Compositions of the Samples

Nominal Composition	Component	% by weight
Be_3N_2	Be_3N_2	94.60
	BeO	4.86
	Be(metal)	0.37
	C	0.05
	ℓ	0.05
	Cr	0.01
	Fe	0.05
	Mn	0.01
	Total	100.00
$BeO \cdot A\ell_2O_3$	$BeO \cdot A\ell_2O_3$	96.77
	$A\ell_2O_3$ (excess)	3.23
	Total	100.00

Experimental Procedure

The enthalpy measurements were made by the "drop" method using a precision Bunsen ice calorimeter. In brief the method, which has been described in detail in a previous publication [2], is as follows. The sample, enclosed in a suitable container, is suspended within a thick-wall silver pipe in a furnace until it comes to a constant, known temperature. It is then dropped, with nearly free fall, into the ice calorimeter which measures the heat evolved by the sample plus container in cooling to 273.15°K. In order to account for the enthalpy of the container itself and the heat lost during the drop, a similar experiment is made with the empty container at the same furnace temperature. The difference between the two values of heat is a measure of the enthalpy change of the sample between 273.15°K and the temperature in the furnace.

In making the measurements reported in this chapter the temperature of the sample in the furnace was in each case measured independently by two Pt-10% Rh thermocouples calibrated at NBS. Because the simultaneous readings of these two thermocouples systematically disagreed by amounts up to about 1°, a comparison was later made with a third calibrated thermocouple which agreed closely with one of the first two and confirmed the suspicion that the other, older thermocouple had undergone slight changes since its last calibration. The Be_3N_2 sample was in a container composed mostly of the alloy 80% Ni-20% Cr, and subsequently the same empty container was measured in order to preclude possible small differences in composition and oxide coating of two different containers. The $BeO \cdot Al_2O_3$ sample was in a sealed container mostly composed of pure silver, and the empty-container values used here were those measured on a similar container of identical mass of parts in previous work in this laboratory [3].

The Be_3N_2 sample was loaded into its container in an efficient dry box, and the container was deliberately kept not quite gas-tight in order to allow the escape of any gas (H_2O or NH_3) unknowingly present. Although the gas space in the container was filled with helium and an effort was consistently made to keep out air and moisture, the sample alternately lost and gained a few tenths percent in mass during the first few runs. This behavior probably accounts for the lower percentage of Be_3N_2 in the final sample than expected. These preliminary runs were discarded, and only those made after the sample had reached nearly constant weight were used in obtaining the final smoothed results represented by equation (1) below.

Results

The observed heats and derived net enthalpies from individual runs are recorded in Table 2 for Be_3N_2 and in Table 3 for $BeO \cdot Al_2O_3$. All values in these tables have been corrected for the impurities (assumed to be separate phases) according to the compositions in Table 1. These heat corrections were computed from Kelley's compilation [4] except that the major corrections for BeO and Al_2O_3 were computed from tables based on recent accurate NBS work [5].

Table 2

Enthalpy Measurements[a] on Beryllium Nitride (Be_3N_2)

Furnace temperature[b] t°C	Measured Heat			Enthalpy Change of Be_3N_2 [c]			
	Empty container, cal	Mean Empty container, cal	Container plus Be_3N_2, cal	Mean observed cal/mole	Calc. eqn.(1) cal/mole	Mean observed minus calculated cal/mole	Difference (% of calculated)
99.9	160.48 161.01 159.57 159.59 160.97 160.61	160.37	267.05 267.59 267.63	1662.9	1660.7	+ 2.2	+ 0.13
199.7	332.61 332.35	332.48	573.55 573.52	3744.3	3752.3	- 8.0	- 0.21
299.6	509.57 509.50	509.54	905.81 905.91	6156.1	6143.9	+12.2	+ 0.20
399.5	695.62 694.11 693.95	694.56	1255.5 1257.0 1255.4	8720.7	8728.0	- 7.3	- 0.08
499.2	882.21 882.76 883.79 883.97	883.19	1619.2 1619.8 1620.4	11442.	11439.	+ 3.	+ 0.03
599.4	1079.88 1079.17 --- ---	1079.5	1997.7 1997.2 1995.9 1997.8	14254.	14263.	- 9.	- 0.06
699.7	1287.54 1288.19	1287.9	2394.4 2393.8	17183.	17170.	+13.	+ 0.08
799.8	1506.07 1505.31 ---	1505.7	2801.7 2801.7 2802.3	20134.	20141.	- 7.	- 0.03
899.9	1726.10 1726.87 1726.83 ---	1726.6	3217.1 3218.7 3220.0 3219.3	23178.	23177.	+ 1.	0.00

[a] Impurity corrections have been applied to data listed here.

[b] International Temperature Scale of 1948, as modified in 1954.

[c] Corrected mass of beryllium nitride, 3.5434g.

Table 3

Enthalpy Measurements[a] on Beryllium Aluminate ($BeO \cdot A\ell_2O_3$)

Furnace temperature[b] t°C	Measured Heat		Enthalpy Change of $BeO \cdot A\ell_2O_3$ [d]			
	Empty container[c] cal	Container plus $BeO \cdot A\ell_2O_3$ cal	Mean observed cal/mole	Calc. Eq.(2) cal/mole	Mean observed minus calculated cal/mole	Difference (% of calculated)
99.9	74.00	188.11 186.64 187.21	2638.3	2639.0	- 0.7	- 0.03
199.7	150.18	400.99 401.33	5843.4	5846.1	- 2.7	- 0.05
299.6	227.52	630.53 629.49	9370.9	9363.5	+ 7.4	+ 0.08
399.5	306.41	868.15 868.27	13080.	13080.	0.0	0.00
499.2	387.06	1113.3 1114.5	16923.	16932.	- 9.	- 0.05
599.4	469.14	1366.9 1368.1	20916.	20916.	0.	0.00
699.7	554.24	1628.6 1627.8	25004.	24997.	+ 7.	+ 0.03
799.8	641.33	1892.9 1892.9 1892.8 1894.4 1893.2	29148.	29149.	- 1.	0.00
899.9	731.57	2165.2 2164.7 2164.6	33369.	33370.	- 1.	0.00

[a] Impurity corrections have been applied to data listed, primarily for 3.23% free $A\ell_2O_3$.

[b] International Temperature Scale of 1948, as modified in 1954.

[c] Each value given is the mean of two or more empty-container experiments performed several years ago.

[d] Corrected mass of beryllium aluminate, 5.4535 g.

The corrected net relative enthalpies of the two substances were smoothed by fitting the mean at each temperature (given equal weight) by the method of least squares to several alternative empirical functions of temperature, using an IBM 7090 computer. For each substance the equation adopted was selected to meet three criteria:

(a) The absence of points of inflection not commonly found for solids showing no transitions (since the data indicate no transitions in the temperature range of the measurements);

(b) The best fit to the observed values fit consistent with the precision of the data; and, for convenience,

(c) An equation which would provide a plausible extrapolation up to the melting point. (Most known heat capacities of solids increase steadily with temperature, and approach within a few percent of the heat capacity of the liquid at the melting point.) The adopted equations are (in cal mole^{-1} deg K^{-1} at T°K, where 1 cal = 4.1840 joules):

$\underline{Be_3N_2(c)}$:

$$C_p = 15.9905 + 7.643(10^{-3})T + 11808.5/T - 6.8143(10^6)/T^2 + 9.0608(10^8)/T^3 \quad (1)$$

$\underline{BeO \cdot Al_2O_3(c)}$:

$$C_p = 42.8895 + 2.856(10^{-3})T - 4309.1/T - 1.27(10^8)/T^3 \quad (2)$$

The "calculated" values in Tables 2 and 3 are those given by these equations (after integration).

Comparison with Previous Work

So far as the authors know, the only other measurements of the enthalpy and heat capacity of these substances previously reported are: Be_3N_2, by Sato [6], 273°-773°K; $BeO \cdot Al_2O_3$, by Nilson and Pettersson [7], 273°-373°K. These results are summarized by Kelley [4]. Compared with the authors' smoothed heat capacities given by equation (1) above, Sato's heat capacities for Be_3N_2 (as calculated by Kelley) are lower by about 3% at 500°K and higher by about 7% at 700°K. Nilson and Pettersson's heat capacity for $BeO \cdot Al_2O_3$ is lower by about 3.7%.

Comparison of the Heat Capacity of $BeO \cdot Al_2O_3$ with that of an Equimolar Mixture of BeO and Al_2O_3

The NBS measurements on the two oxides BeO and Al_2O_3 [2,5], made with the same apparatus over the same temperature range as on $BeO \cdot Al_2O_3$, gives an approximate answer to the question of how nearly the heat capacity of the double oxide approaches that of its two uncombined component oxides at each temperature. These deviations from additivity on this basis are tabulated in Table 4. The deviations are surprisingly small — so small, in fact, that they are uncertain by at least half their magnitudes considering the combination of experimental errors involved in measuring the three substances. From the microscopic examination of the $BeO \cdot Al_2O_3$ sample noted earlier in this chapter, it seems safe to assume that most of the sample was $BeO \cdot Al_2O_3$. Even if 20% of the sample (corresponding to the unidentified voids observed) were unreacted BeO and Al_2O_3, the error in each heat-capacity value of $BeO \cdot Al_2O_3$ reported in this chapter <u>arising from this source</u> would amount to some small fraction (of the order of 20%) of the small percentage deviations from additivity in Table 4.

Table 4

Deviations of the Heat Capacities of $BeO \cdot A\ell_2O_3$ from the Sum of those of the Component Oxides

Temperature T (°K)	C_p (cal mole^{-1} deg K^{-1})				ΔC_p, $BeO \cdot A\ell_2O_3 - BeO - A\ell_2O_3$[b]	
	BeO[a]	$A\ell_2O_3$[a]	Sum	$BeO \cdot A\ell_2O_3$ (equation (2))	cal mole^{-1} degK^{-1}	%
300	6.148	18.979	25.127	24.679	- 0.45	-1.8
400	8.083	22.986	31.069	31.275	+ 0.21	+0.7
500	9.310	25.345	34.655	34.683	+ 0.03	+0.1
600	10.128	26.889	37.017	36.833	- 0.18	-0.5
700	10.714	27.969	38.683	38.363	- 0.32	-0.8
800	11.154	28.758	39.912	39.540	- 0.37	-0.9
900	11.498	29.354	40.852	40.498	- 0.35	-0.9
1000	11.776	29.814	41.590	41.310	- 0.28	-0.7
1100	12.005	30.176	42.181	42.018	- 0.16	-0.4
1200	12.197	30.464	42.661	42.652	- 0.01	-0.0
1300	12.361	30.695	43.056	43.230	(+ 0.2)	(+0.4)
1400	12.503	30.881	43.384	43.764	(+ 0.4)	(+0.9)
1500	12.628	31.032	43.660	44.263	(+ 0.6)	(+1.4)
1600	12.738	31.153	43.891	44.735	(+ 0.8)	(+1.9)
1700	12.836	31.251	44.087	45.184	(+ 1.1)	(+2.4)
1800	12.925	31.328	44.253	45.615	(+ 1.4)	(+3.0)
1900	13.005	31.389	44.394	46.030	(+ 1.6)	(+3.6)
2000	13.078	31.436	44.514	46.431	(+ 1.9)	(+4.1)
2100	13.145	31.470	44.615	46.822	(+ 2.2)	(+4.7)

[a] From NBS Report 6928, Tables B-2 and B-8.

[b] Parenthesized differences are for temperatures beyond the range of measurement.

Derivation of Tables of Thermodynamic Functions

A new sample of $BeO \cdot Al_2O_3$ whose chemical analysis shows much closer to the theoretical ratio of the two component oxides has recently been received. If structure tests of this sample not yet made show it to be much more nearly single-phase, measurements will be made of its relative enthalpy at two or more high temperatures to compare with the results reported here. As mentioned in Part A, Section 3, of this report, precise low-temperature heat-capacity measurements are now in progress on Be_3N_2 and are expected to begin soon on $BeO \cdot Al_2O_3$. When these results become available, they will be combined smoothly with the NBS high-temperature results to give tables of thermodynamic functions from 0°K to high temperatures.

Meanwhile provisional tables have been generated by digital computer for Be_3N_2 and $BeO \cdot Al_2O_3$ from equations (1) and (2), and are given in Appendix B of this report. In each table the entropy and free energy have deliberately been expressed as functions of the undetermined parameter $S^o_{298.15}$, in order to avoid associating estimated (and hence inaccurate) values of this parameter with a table based on precise measurements, and also to anticipate the availability of a Third-Law entropy within the next few months. This new table for Be_3N_2 should supersede the less accurate estimated table given in earlier reports [8], but is based on the same assumed heat of fusion and liquid heat capacities.

Values of entropies and free energies may of course be obtained from the present tables by assuming a value of $S^o_{298.15}$ for the compound in question. For this purpose, tentative estimates are given here. In the case of Be_3N_2, the use of equation (1) at the lower temperatures and the assumption of the Lindemann-Magnus approximation (C_p-C_v proportional to $T^{3/2}$) led to an approximate Debye temperature of 1185°K, and the Debye function then gave

$$S^o_{298.15} = \int_0^{298.15} (C_v/T)\,dT + \int_0^{298.15} [(C_p-C_v)/T]\,dT = 7.9 + 0.2$$

$$= 8.1 \text{ cal/mole-deg K.}$$

(Kelley's estimate of 12 cal/mole-deg K was used in the earlier tables [8].) The lower value estimated here seems not unreasonable, but assumes of course that the isotropic Debye function holds approximately up to 600°K. In the case of $BeO \cdot Al_2O_3$, the best tentative estimate seems to be the sum of the entropies of BeO and Al_2O_3 [5]:

$$S^o_{298.15} = 3.376 + 12.174 = 15.55 \text{ cal/mole-deg K.}$$

According to the transpiration experiments of Young [9], the free-energy change for the reaction

$$BeO(c) + A\ell_2O_3(c) = BeO \cdot A\ell_2O_3(c)$$

is $\Delta G^{o} = -3.2 \pm 1.0$ kcal at 1673°K. From this value and the free-energy functions for $BeO \cdot A\ell_2O_3$ (Appendix B of this report) and for BeO and $A\ell_2O_3$ [5] is calculated $\Delta H^{o}_{298.15} = -3.3$ kcal. if the above tentative assumption be made that $\Delta S^{o}_{298.15} = 0$. (From the same equilibrium data, $\Delta H^{o}_{298.15} = -4.0$ kcal. was previously estimated [10].)

References

1. S. M. Lang, C. L. Fillmore, and L. H. Maxwell, "The System Beryllia-Alumina-Titania: Phase Relations and General Physical Properties of Three-Component Porcelains," J. Research Natl. Bur. Standards 48, 298-312 (1952).

2. G. T. Furukawa, T. B. Douglas, R. E. McCoskey, and D. C. Ginnings, "Thermal Properties of Aluminum Oxide from 0° to 1200°K," J. Research Natl. Bur. Standards 57, 67-82 (1956).

3. T. B. Douglas and A. W. Harman, unpublished work.

4. K. K. Kelley, U. S. Bureau of Mines Bulletin 584: "Contributions to the Data on Theoretical Metallurgy. XIII. High-Temperature Heat-Content, Heat Capacity, and Entropy Data for the Elements and Inorganic Compounds," U. S. Govt. Printing Office, Washington, 1960.

5. NBS Report 6928, Tables B-8 and B-2 (National Bureau of Standards, Washington, D. C., 1 July 1960).

6. S. Sato, "The Specific Heats of Beryllium Nitride, Phosphorus Nitride, and Titanium Nitride," Sci. Papers Inst. Phys. Chem. Research (Tokyo) 34, 888 ff (1938).

7. L. F. Nilson and O. Pettersson, "Über Molekularwärme und Molekularvolumina der seltenen Erden und deren Sulfate," Ber. chem. Gesell. 13, 1459 ff (1880).

8. NBS Report 6645, Table 2-29, 1 January 1960 (amended 1 April 1960); NBS Report 6928, Table B-29, 1 July 1960 (National Bureau of Standards, Washington, D. C.).

9. W. A. Young, "The Reactions of Water Vapor with Beryllia and Beryllia-Alumina Compounds," J. Phys. Chem. 64, 1003-1006 (1960).

10. NBS Report 7192, p. 86, 1 July 1961 (National Bureau of Standards, Washington, D. C.).

CHAPTER B-4

EXPERIMENTAL INVESTIGATION OF THE VAPORIZATION OF SELECTED SUBSTANCES

by J. Efimenko, J. J. Diamond, R. F. Walker,
A. L. Dragoo and N. J. Carrera

I. Introduction

Part of the overall program has been devoted to the development, evaluation, and application of experimental techniques for studying a variety of properties associated with the vaporization of selected substances at high temperature. The aim of the techniques is to determine the principal net reaction, the equilibrium partial pressures of the gaseous species, and the thermodynamics of the vaporization processes, and also to measure rates of "free" evaporation in a vacuum and in the presence of foreign gases. The basic systems selected for investigation are the Be-O-F and the Al-O systems.

This chapter gives details of the techniques which have been used or are under various stages of development and presents some early results of the measurements and observations. The equilibrium-type experiments have all been devoted to the Be-O-F system and are being carried out using a mass spectrometric technique. The kinetic studies have been devoted to the Al-O system, for which a variety of techniques are being employed. The following description of the work is presented in terms of the chemical systems being studied.

II. Mass Spectometric Investigation of the BeF_2 and BeO Systems

Previous NBS Reports (Nos.6297, 6484, 6928, 7093, 7437) have discussed various aspects of the measurement of the vapor pressures and determination or estimation of associated thermodynamic data for the BeF_2 and BeO systems. The BeF_2 system has been studied only cursorily with the mass spectrometer, and all but one of the previous investigations have employed either the Knudsen effusion or the transpiration techniques. The important vapor species in this system have not, therefore, been clearly identified under extreme conditions. The vaporization of BeO has been studied using both the mass spectrometic technique and the Knudsen technique. A tungsten cell was used for the mass spectrometric study, and it is one of the aims of the present investigation to check the previous results and employ cells composed of other refractory metals to determine the reducing effect of metals on oxides. Vaporization in the two component system BeF_2-BeO has not been studied previously, nor is a constitution diagram of the condensed system available. The widely different melting points and volatilities introduce more difficult experimental problems into the the study of the two component system than are present when the components are investigated individually.

Apparatus and Technique

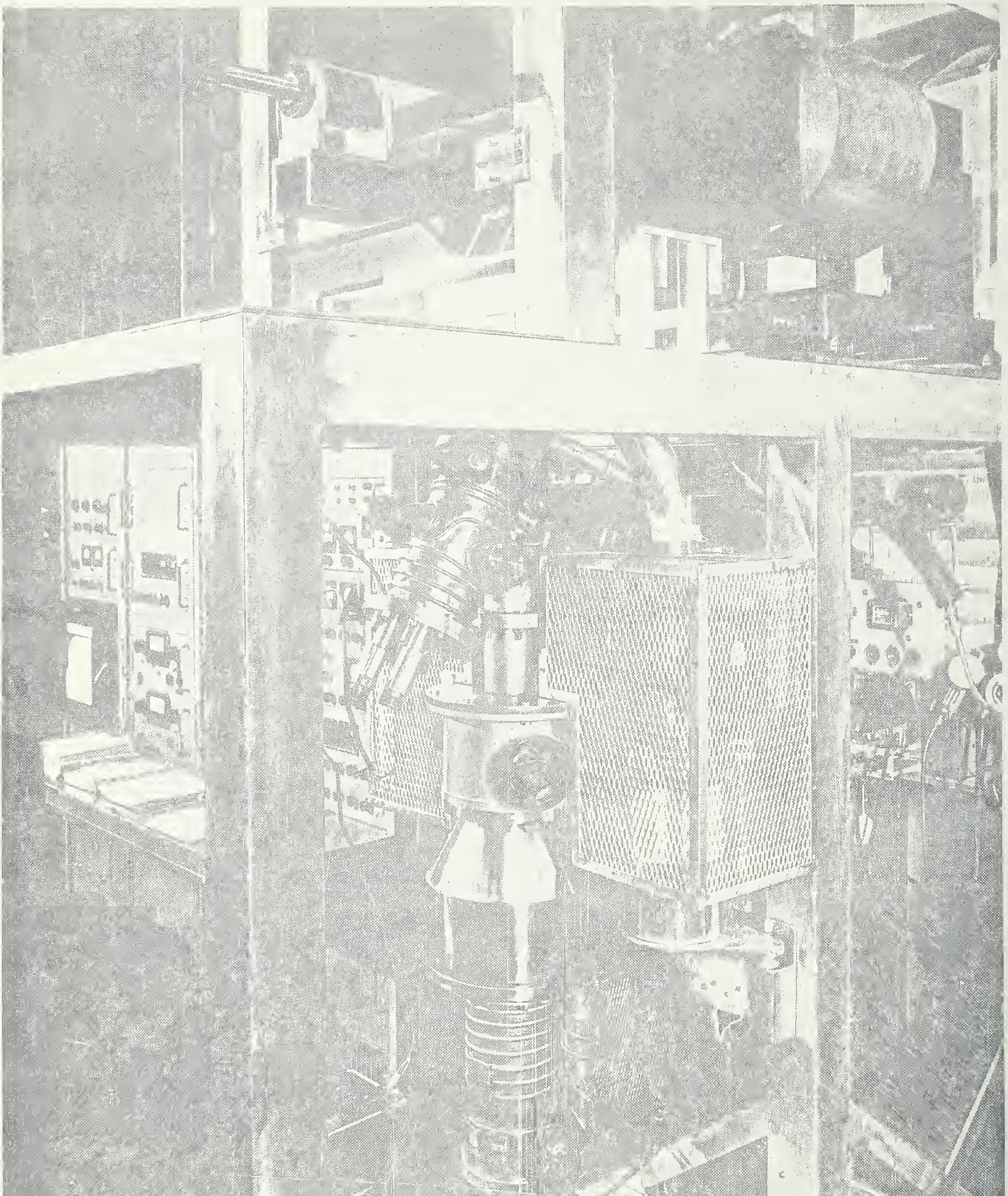
The basic instrument in use for this part of the investigation is a 12in. radius, 60° sector, directional focusing mass spectrometer, constructed by Nuclide Analysis Associates following the design of M.Inghram. The Knudsen cell chamber, ion source, and analyzer tube are each pumped independently in this particular instrument, a 6in., 600 liter/sec, Edwards mercury vapor pump being used to evacuate the cell region. (Figure 1). As shown in the figure, this pump has associated with it a metal liquid nitrogen trap and valve, which are unfortunately assembled with neoprene gaskets and a grease seal, instead of gold gaskets as in the rest of the system. The neoprene and grease contribute to a rather high background spectrum, and modification of this part of the pumping system will be undertaken as soon as convenient. It is planned to eliminate the valve, introduce a cooled baffle between the pump and cold trap, and modify the flanges to take gold gaskets. A second mechanical pump, backing up the Edwards pump alone, has already been introduced with some improvement to the background. In order to distinguish background species from the ones originating in the Knudsen cell, a shutter positioned between the Knudsen cell and ionization source can be interposed across the molecular beam during an observation.

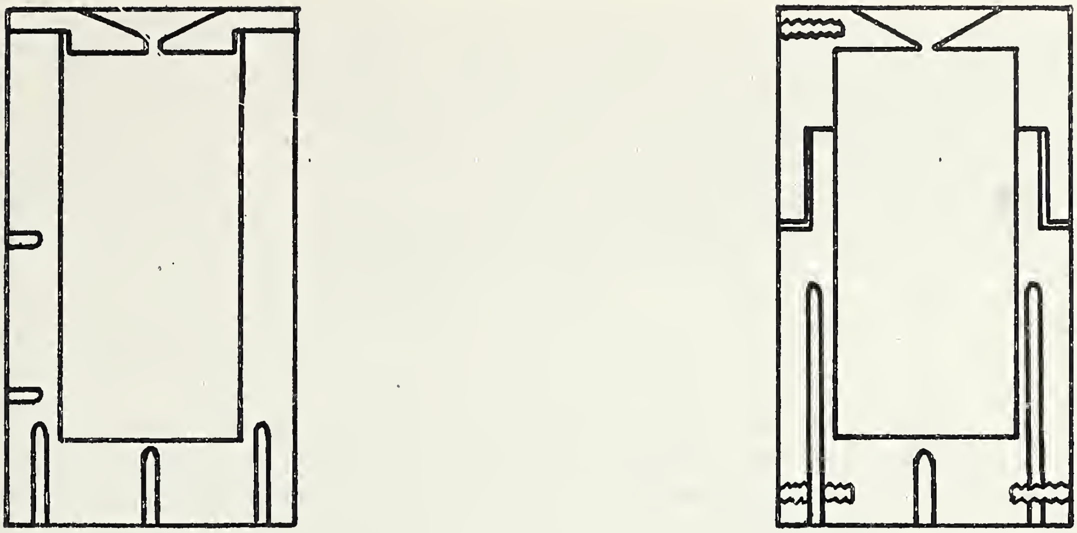
Apart from the residual gases, a major problem that has arisen with the apparatus has been a tendency for the Knudsen cell support to sag at temperatures in excess of 1600°C. This support sagging problem arises from the geometry of the analyzer tube position and the attached Knudsen cell mounting. The Knudsen cell is mounted coaxialy on the analyzer tube which sets at an angle of 30° to the vertical. As a consequence the molecular beam effusing from the cell became misaligned with respect to the slit which admits the beam to the source region, and quantitative measurements of the relative abundance of the different vapor species at various temperatures were impeded. This high temperature alignment problem could be solved by orienting the analyzer tube and, therefore, the Knudsen cell to a vertical position. However, such a change would involve too long a shut-down period. An alternative solution has been to strengthen the support system. The support system is attached directly to the flange shown at the bottom of the Knudsen cell chamber in Fig. 1. Major changes to improve the stability of the support are as follows: four glass insulation legs which were used to attach the support system to the flange have been replaced with stainless steel rods except for about one inch length of glass, retained for electrical insulation; the thickness of the mounting plate has been doubled. The depth of the support rod holes in the bottom of the Knudsen have been deepened to increase stability. As a result of these changes, preliminary test runs have indicated that a temperature of 2000°C can be attained using the original, heavy-type cell without any detectable distortion of the support system. Further tests to higher temperatures will now be made.

Figure 1

Chamber housing the Knudsen Cell, with 6 in. mercury diffusion pump mounted below. 'A' identifies the flange upon which the Cell is mounted at an angle of 30° to the vertical.

(See next page.)





OLD DESIGN

NEW DESIGN

FIG. 2 KNUDSEN EFFUSION CELL

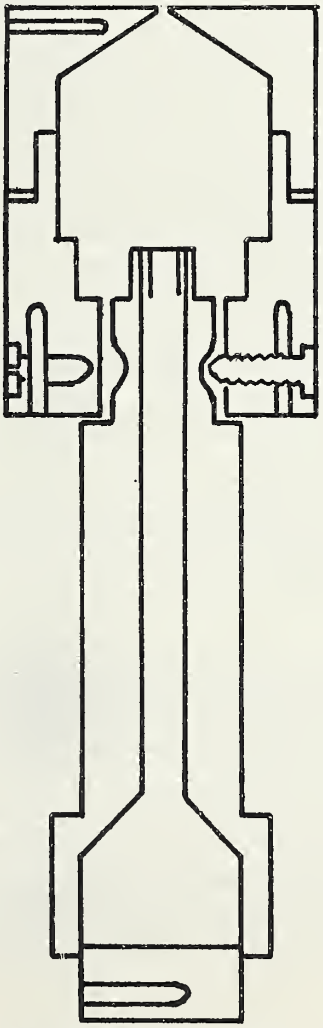


FIG. 3 TEMPERATURE GRADIENT EFFUSION CELL

Another serious problem arose from the difficulty of accurately measuring and maintaining a uniform temperature in the cell. This problem was particularly severe at low temperature (< 1000°C) when the cell was heated by radiation only, from hotter tungsten filaments. Initially, the design of crucible shown in Figure 2 was heated by radiation and electron bombardment from a single tungsten filament. At least partial solution of the problems has been obtained by using a new design of cell, also shown in Figure 2, and by heating the upper and lower halves of the cell with two separate filaments. Additional black body holes were also included in the new design to permit temperature gradients along the wall of the cell to be more reliably surveyed with an optical pyrometer sighting through a window in the side of the cell chamber. An additional window with magnetically operated shutter has been installed in the bottom flange of the cell chamber, in order that the bottom of the cell can be viewed with a second optical pyrometer. Various types of thermocouple are also being explored for temperature measurement purposes.

Tungsten and molybdenum cells have been used so far, but iridium and rhenium cells are currently under-construction. For the preliminary investigation of the BeF_2 and BeO systems, the materials were placed directly inside the tungsten cell. In studying the BeF_2-BeO system it was soon found that at temperatures high enough to detect vapor species from the BeO component, the BeF_2 supply was rapidly depleted. A temperature gradient cell has, therefore, been designed and fabricated, and its potentialities are being investigated. The general design is illustrated in Figure 3; it is intended that BeF_2 vaporizing at a relatively low temperature in the bottom chamber of the cell will react with the BeO contained in the upper chamber at a higher temperature. The upper chamber will be heated by electron bombardment while the lower chamber will be heated by thermal conduction along the walls of the tube connecting the two.

More complete details of all the above design changes will be described in later reports when their effects have been more thoroughly evaluated.

Results

The following is a summary of results, obtained for the most part before the changes discussed above were contemplated. It is anticipated that as a result of changes many of the observations can now be placed on a firmer quantitative basis.

Investigations of the BeF_2 were further complicated by the poor crystallinity and presence of water vapor in the available samples. Above 400°C BeF_2 was the principal vapor species detected and the variation of its intensity as a function of temperature was followed both above and below the melting point. In the temperature range 400-660°C the following mass numbers (m/e) were detected: 9, 19, 20, 28, 47, (64), 66, 75, and 85. Most of the numbers were attributed to specific species. No interaction between BeO and BeF_2 heated together in a tungsten effusion cell was observed but the temperature was not high enough to cause any sensible evaporation of the BeO itself. When BeO alone was heated in the cell, mass 9 (Be^+) was observed at 1700°C, masses 25 (BeO^+) and 75 ($(BeO)_3^+$) were observed in the range 1800-1900°C, but at 2400°C large intensities of Be^+ and O^+, and some BeO^+ were apparently formed independently of the ionizing electrons in the source region. The observations in the 1700-1900°C range are in agreement with those of Chupka and coworkers who used a closely similar technique. However, the effect observed at 2400°C raises disturbing questions as to the extent to which a similar occurrence may have affected their reported results.

III. Rate of Vaporization of Aluminum Oxide

The background of previous experimental research on the vaporization of aluminum oxide has been presented in previous NBS Reports (Nos. 6297, 6484, and 6928). Most of the previous work has been concentrated on establishing the principal net reaction and the thermodynamics of vaporization under neutral or reducing conditions, by studying the vaporization from Knudsen cells. The present work has the initial aim of studying the rate of "free" vaporization in a vacuum, in order to determine if the vaporization coefficient is significantly different from unity for either the solid or liquid oxide; of comparing the rates of evaporation in the presence of different foreign gases; and determining some of the properties of the condensed vapors. Subsequent identification of the vapor species under equilibrium conditions and under the conditions of "free" vaporization are also planned.

The simplest method of determining the vaporization coefficient is to compare the free vaporization rate with absolute effusion rates from a Knudsen cell. For this purpose the effusion measurements of Brewer and Searcy [1] are probably the best available. By this method Sears and Navias [2] arrived at the conclusion that the coefficient of the solid oxide is about 1/4000, but their technique was not ideal, and the conclusion is based on somewhat tenuous arguments. During the course of their mass spectrometric study of the vapor effusing from a tungsten cell, Drowart, DeMaria, Burns, and Inghram [3] observed that the effusion hole became clogged with liquid alumina, but that neither the relative nor absolute intensities of the vapor species changed as a consequence. These results indicate that the vaporization coefficient of liquid alumina is close to unity. Furthermore, they indicate that the composition of the vapor freely evaporating from the oxide surface is identical with that of the equilibrium vapor.

Measurements of the rate of vaporization in vacuo are complicated by the difficulty of heating the oxide to high temperatures without introducing effects due to the presence of an external heating element. Although suitable heating techniques can be devised in principle, they introduce more than usually severe problems of temperature measurement and control. Furthermore, if the rates are to be measured in the presence of an oxidizing gas, all available heating elements would be rapidly consumed above 1750°C. New techniques and evaluations have, therefore, been devised in an attempt to cope with these problems.

Experimental Techniques

1. Microbalance Technique

Conducting samples may be suspended from a microbalance in a vacuum, and their rates of vaporization may be measured by heating the samples of known surface area directly by induction. Attempts to adapt this technique to measurements on alumina by enclosing the sample in tubular susceptors of platinum, molybdenum, or tungsten did not prove very reliable, as significant quantities of the metals were transported to the sample or its suspension. A technique was, therefore, developed whereby a rod of tungsten was vacuum-sealed inside a tube of alumina with the aid of an arc image furnace. The technique still requires considerable improvement to increase the precision of the results obtained, but in its present state of development it appears to yield results which are correct within an order of magnitude.

Figure 4 illustrates the general form of the samples and their method of suspension from the microbalance. One end of a tube of Morganite alumina, approximately 1/8 in. O.D. x 0.02 in. wall thickness x 1 in. long, was melted in air with an arc image furnace until about 1/8 in. of the tube had been closed with the molten material. This end was then ground to a diameter uniform with that of the tube, and an 0.010 in. dia. suspension hole was drilled through the fused material along a diameter, by means of an ultrasonic drill. A piece of tungsten rod, approximately 3/4 in. long x 0.080 in. dia. was next inserted in the tube. The other end of the tube was then closed by forming a neat hemispherical cap of molten material in the arc image furnace, after first evacuating the tube in a pyrex bulb.

The dimensions of the tungsten rod were determined by two factors: its diameter had to be large enough to permit efficient coupling with an induction field in order to obtain high temperatures; on the other hand its weight had to be restricted, if the sensitivity of the microbalance was to remain high enough to detect significant weight changes during short runs.

The samples were attached to the microbalance with an 18 in. chain of 0.010 in diam. sapphire single crystal rods. The lowest rod was fused together in sections to support the sample with its axis vertical, as shown in Figure 4.

The Morganite alumina used for the tubes was not as pure as initially desired (see below for a typical analysis), but it had the advantage of being readily available in the desired shape, and was dense and reasonably opaque.

The high density was desirable, because it was hoped to confine any effects arising from the presence of the tungsten to those resulting from diffusion of tungsten through the oxide. However, as a result of rapid heating and cooling of the samples it was inevitable that the oxide

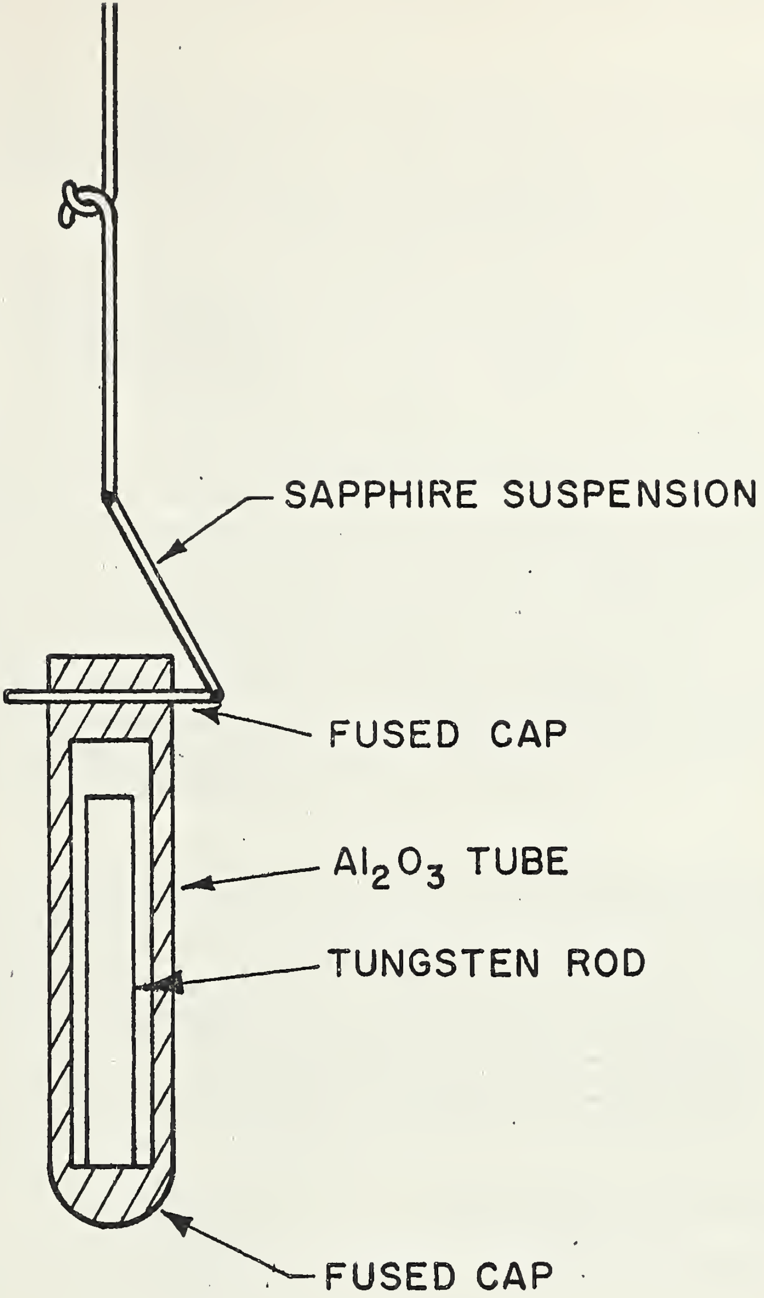


FIG. 4 Al_2O_3 SAMPLE USED FOR MICROBALANCE MEASUREMENTS would ultimately crack from thermal stresses. After a few runs on the same sample, this did in fact occur; no significant trends in the data were observed as a consequence, but the cracks contributed to a severe problem of accurate temperature measurement.

The temperature of the vaporizing surface was estimated from observations with an optical pyrometer, adjusted for emittance, window absorption, and angle of sighting. In the arrangement used here, the possibility exists that the observed temperatures were systematically too high, because of the presence of the hotter tungsten inside the sample. Errors from this effect are believed to be small, however, in comparison with those which arose from variations in the brightness of surface. The closed ends of the samples were much cooler than the central 0.8 in. and were not included in the calculation of the vaporizing area. More important, however, was the mottled appearance which the surface took on at high temperature, particularly with the second of the two samples used for the measurements. The mottling made it difficult to obtain a good match with the pyrometer; this problem was increased during later runs when cracks in the surface contributed further to discontinuities in the surface brightness. In the worst instances these problems contributed to an uncertainty of ±50°C in the observed brightness temperature, although with the first sample employed the uncertainty was more nearly ±10°C.

The microbalance and experimental procedure employed were similar to those previously described [4]. The sample was heated rapidly to a high temperature, held at this temperature until the sample was estimated to have lost at least 100 micrograms, and then cooled rapidly. The weight change was determined to the nearest microgram (with an uncertainty of ±3 micrograms) from observations of the position of the microbalance beam before and after heating. Displacements of the beam were calibrated using Class M microbalance weights obtained from the NBS Mass and Scale Section.

2. Reimaging Furnace Technique

Reimaging an incandescent source onto the surface of a substance under investigation can provide a ready means of heating it locally to a high temperature. The particular advantage of this technique as applied to alumina is that it permits heating in reducing, neutral, or oxidizing atmospheres without the occurence of side reactions associated with the presence of a conducting crucible or heating element. As with the foregoing technique, there are also severe problems of accurate temperature measurement, and these are combined with some uncertainty as to the effective vaporizing area. Nevertheless, under suitably restricted conditions it has been found possible to obtain useful information with the technique, and to draw quantitative conclusions within broad, but defined limits of uncertainty.

A modified A. D. Little reimaging furnace is the basic tool being used for this part of the program. Essentially, the technique in use involves concentrating the image of a carbon arc onto one end of a 1/8 in. or 1/4 in. rod of Morganite alumina. By enclosing the rod in a pyrex bulb, evacuating the bulb, and making provision for the admission of any desired gas, rates of vaporization may be measured by weighing on a microbalance before and after heating. Since temperature gradients away from the heated end of the rod are very steep, only the directly heated end is considered in determining the effective vaporizing area. Measurements and observations have thus far only been carried out on liquid alumina. The alumina rod has been held horizontal, so that when the heated end is melted, a slightly pendant drop of the liquid is formed on the end of the rod. Estimation of the surface area of this drop introduces an uncertainty in the measurements of the rate of vaporization. It would be quite feasible to hold the rod vertically, and thus estimate more precisely the surface area of the more symmetrical drop that would be formed. However, the uncertainty in the temperature is also another possible major source of error, and it is not yet clear which of the two sources of error is the more important.

Temperatures are measured with an optical pyrometer, sighting at the heated end along the axis of the rod. Measurements are made under conditions such that the reflected-energy area is avoided, and a spectral emissivity of one can be assumed [5].

Owing to its good infrared transmitting properties, single crystal alumina could not be melted with the furnace. The polycrystalline material melted readily, however. It is believed that the molten material also absorbs very little of the incident radiation from the arc, so that increasing the amount of energy incident on the liquid serves to increase the size of the molten drop rather than increase its temperature. As a consequence, it has not been possible to cover a wide temperature range during the measurements; on the other hand, fluctuations in the output of the arc resulted in smaller fluctuations in the liquid temperature than might otherwise have been the case. Furthermore, fluctuations in the output tended to vary the size of drop and contributed to the problem of defining the effective vaporizing area. Nevertheless, temperature fluctuations of about ±25°C were normally observed during the course of a run. The duration of runs was limited to about 20 minutes, the time taken for the arc to consume one anode.

The technique permits the collection of the vapor on the cold wall of the flask or on a pyrex slide held within the flask. In a vacuum, the condensate collects as a thin transparent film, while in the presence of another gas convection currents tend to carry the vapor to the top of the flask. In neither case, therefore, do changes in the transmissivity of the flask seriously affect the optical pyrometer measurements.

Purity of Alumina Samples

The process of conducting various experiments on liquid alumina involved keeping it molten, held on a rod of solid alumina by surface tension, for a total time of about an hour. During this period a variety of oxidizing, reducing and inert atmospheres surrounded the molten sample. A substantial purification of the material was found to occur. The original Morganite alumina was found by semi-quantitative spectrochemical analysis to contain 0.01 to 0.1% each of Fe, Ga and Si and 0.001 to 0.01% each of Mg, Ti and Zn, with lesser amounts of Ca, Cu, Cr, Mn and V. After purification in the image furnace, the alumina contained no contaminants in the 0.01 to 0.1% range, Fe, Mg, Si and Ti in the 0.001 to 0.01% range and lesser amounts of Ca and Cu. Cr, Ga, Mn, V, and Zn were no longer detectable. It is estimated that the alumina content of the specimen was increased from an initial 99.7% to about 99.95%.

Results

1. Rate of Vaporization in a Vacuum

Measured rates of vaporization of solid Al_2O_3 using the vacuum microbalance technique are summarized in Table I. For comparison purposes only, the rates have been converted to vapor pressures assuming AlO is the vaporizing species and that the vaporization coefficient is unity. The vapor pressures are plotted in Figure 5, where they are compared with the Knudsen cell measurements of Brewer and Searcy on liquid alumina, which also assume AlO is the appropriate species. The data of Brewer and Searcy may be represented by:

$$\text{Log } P_{AlO} \text{ (atm)} = -\frac{30014}{T} + 7.886 .$$

This line has been extrapolated in the figure using a heat of fusion of 26 kcal/mole.

It will be observed that there is considerable scatter in the data. This scatter can be entirely accounted for in terms of the ±50°C uncertainty in some of the observed brightness temperatures. Errors devolving from the assumption of a constant emissivity of 0.4 throughout the measurements also contribute an uncertainty of about ±25°C in the reported temperatures. Considering these uncertainties and the fact that the reported pressures of Brewer and Searcy may be high by a factor of 2-4, leads to the conclusion that the results obtained with this technique are not inconsistent with a value of unity for the vaporization coefficient of solid alumina. When all sources of error are considered, the results indicate that the vaporization coefficient must lie in the range 0.1 - 1.0.

There is a conflict between this conclusion and that of Sears and Navias. However, their conclusion was based largely on an estimate of the upper limit of the thickness of an aluminum-oxygen condensate on a glass envelope. Since the condensate was not visible, they estimated that it was not more than 10-20 Å thick, and they used this estimate to determine an upper limit to the rate of vaporization. As discussed below, when the vapor from alumina condenses on a pyrex envelope it does so as a transparent film, which is not visually detectable until interference fringes are observed. Still thicker films may be deposited which cannot be seen until they begin to peel away from the pyrex. These observations

TABLE I

RATE OF VAPORIZATION OF SOLID ALUMINA

TRUE TEMP. °K	TIME mins	WEIGHT LOSS micrograms	RATE OF WEIGHT LOSS g/cm^2/sec	VAPOR PRESSURE as AlO* atm
<u>1st Sample</u>				
1856	60	157	2.13×10^{-8}	2.68×10^{-9}
1861	40	77	1.57×10^{-8}	1.96×10^{-9}
1938	33	255	6.30×10^{-8}	8.05×10^{-9}
<u>2nd Sample</u>				
1844	27	126	3.48×10^{-8}	4.34×10^{-9}
1896	30	62	1.55×10^{-8}	1.96×10^{-9}
1966	20	194	7.25×10^{-8}	9.33×10^{-9}
1990	12	556	3.47×10^{-7}	4.49×10^{-8}
2113	$2\frac{1}{4}$	550	1.83×10^{-6}	2.44×10^{-7}
1948	2	78	2.92×10^{-7}	3.74×10^{-8}
2031	2	28	1.05×10^{-7}	1.37×10^{-8}
1972	2	31	1.16×10^{-7}	1.49×10^{-8}
2042	2	125	4.67×10^{-7}	6.12×10^{-8}
2136	2	215	8.03×10^{-7}	1.08×10^{-7}
2089	2	166	6.20×10^{-7}	8.22×10^{-8}
2149	1	122	9.01×10^{-7}	1.21×10^{-7}
2107	2	321	1.20×10^{-6}	1.60×10^{-7}
2149	2	383	1.43×10^{-6}	1.92×10^{-7}

* Assuming a vaporization coefficient of unity and an emissivity of 0.4

suggest that the condensate in the Sears and Navias experiment could have been at least two or three orders of magnitude thicker than they supposed, in which case there would be no conflict between their observations and the above measurements.

The measurements of the rate of evaporation of liquid alumina using the arc image furnace also show considerable scatter, and sufficient data has not yet been accumulated to attribute the scatter quantitatively to different possible sources of error. It is, however, possible to assign some outside limits of error arising from the principal sources of uncertainty. For example, during a sequence of ten runs in a vacuum of 6×10^{-6} torr and using 1/4 in. diam alumina rods, the measured rates of evaporation varied from 3.58 to 7.15 mg/min. In all instances the observed temperature was in the range 2260±25°C and the effective vaporizing surface was certainly greater than 32 sq.mm and probably less the 63 sq.mm. It is interesting to use these rough figures to determine whether they are suggestive of an evaporation coefficient significantly different from unity. Assuming an evaporation coefficient of unity, and again purely for comparison purposes taking AlO as the vapor species, the range of vapor pressures indicated by the above data is given in

Figure 5. It will be observed that the results obtained so far are not inconsistent with a value of unity for the evaporation coefficient of liquid alumina, and that the value most probably lies in the range 0.1 to 1.

As further experience is gained with the image furnace technique it is anticipated that a considerable increase in precision will be obtainable. For example, a sequence of three of the above runs during which better than usual control of the temperature and, in particular, of the drop size was maintained yielded rates of weight loss which agreed within about 1%. Several procedures are being explored to determine if this precision can be maintained routinely. Solution of the problem of controlling and measuring the effective vaporizing area will enable better estimates to be made of the uncertainty in the temperatures.

2. Vaporization in the Presence of Other Gases

Experiments in the presence of other gases have thus far been restricted to qualitative studies with the arc image furnace designed to indicate the severity of the additional experimental problems that are likely to be encountered. More quantitative studies will follow. It has, however, already been possible to observe some gross changes in the vaporization behavior of molten alumina when exposed to pressures of up to one atmosphere of Ar, He, O_2, H_2, N_2 and H_2O. For example, some evidence for relative rates of vaporization in the different gases can be gained from a visual impression of the amount of deposit on the enclosed flask.

Apart from changes in the effective vaporizing area mentioned in the following paragraph, qualitative impressions may be summarized as follows: A marked increase in the rate of vaporization of alumina was observed in the presence of hydrogen, together with extensive whisker growth at the solid-liquid interface. The solidified material was grey in appearance, and at some ill-defined, but intermediate rate of cooling a "nose" has been observed to grow on the solidifying drop, resulting in a porous solid. This may have been due to the presence of some dissolved gas, but the phenomenon did not appear to be closely associated with the more pronounced effect described below. Observations in the presence of the other five gases were not suggestive of any gross differences in rates of vaporization of liquid alumina, and in all cases the solidified material remained white. (Initially, the relatively impure material acquired a slightly yellow appearance when heated in oxygen, presumably arising from the presence of iron). Heating and cooling in the presence of water vapor resulted in a porous solid.

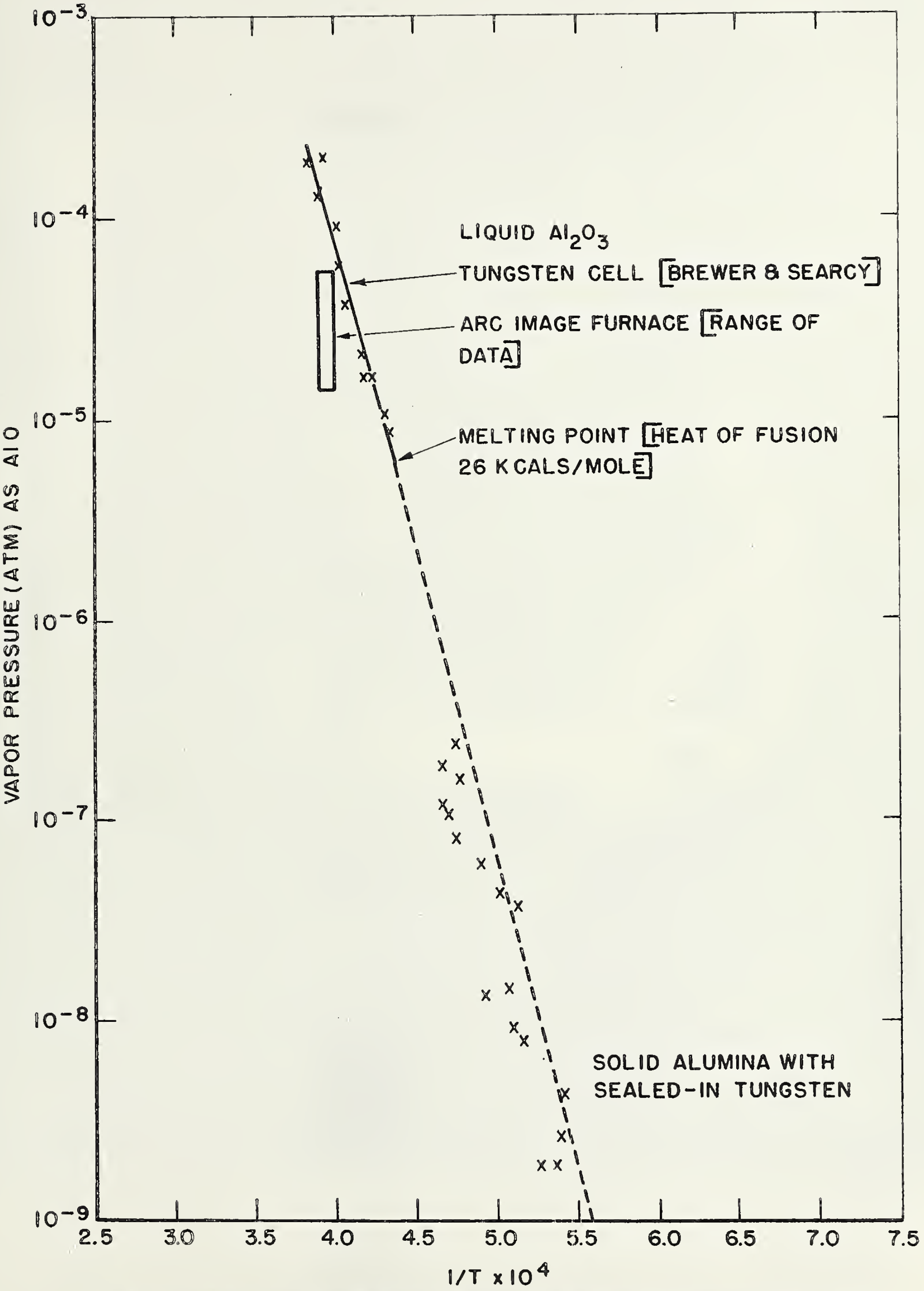


FIG. 5 COMPARISON OF MEASUREMENTS OF RATES OF VAPORIZATION OF ALUMINA, CONVERTED TO VAPOR PRESSURES ASSUMING AlO AS VAPOR SPECIES

Figure 6

Molten drop of alumina in one atmosphere of water vapor, showing bubble (surrounded by white halo) emerging as the drop cools. Photograph taken through an optical pyrometer. The halo, which is not detectable with the eye, appears on all side-view photographs of the bubbles, and is not explained.

When a molten drop of alumina was partly frozen in an atmosphere of water vapor, the remaining liquid was seen to boil vigorously. Partial freezing in an atmosphere of H_2, He, N_2, O_2, Ar or air produced no observable effect. When a water vapor atmosphere around a drop of molten alumina was replaced by one of these gases, or vice versa, the size of the drop was seen to increase or decrease depending on the molecular weight (i.e. heat conductivity of the gas relative to that of H_2O). When H_2O replaced N_2, O_2, Ar or air the drop partly solidified and the remaining liquid alumina was seen to boil, indicative of the speed with which the water vapor was absorbed. When H_2O replaced H_2 or He, resulting in an increase in drop size, no boiling was observed. Figure 6 is a photograph of molten alumina containing a large bubble of gas in the process of boiling out. It is concluded that H_2O is readily absorbed by molten alumina and that it (or some water-alumina reaction product) is more soluble in liquid than in solid alumina.

3. Studies of Films Deposited from Alumina Vapor

It has been observed that alumina vaporized in the presence of a gas in an arc-image furnace is carried by convection to the upper part of the enclosing container and deposited as a white, opaque powder. In a vacuum, however, it deposits as a transparent film, visible only when it attains a thickness in the wavelength-of-light range. Thicker films are a light tan and tend to peel from Pyrex when they attain thicknesses of a 1-5 microns. While it is known from published mass spectrometric work that the major vaporizing species under neutral conditions are atomic Al and O [4], the deposited film is not Al metal, but an amorphous aluminum oxide.

Petrographic examination showed the film to be isotropic, with a refractive index of 1.614. Its surface area was .6 square meters per gram, as determined by N_2 adsorption in B.E.T. equipment. Infrared absorption showed the water band at 2.9μ and several absorption "fringes" due to the specimen film being of the same order of thickness as the wavelength of the incident radiation. In general, the film was completely transparent from 1 to 8μ, the transmission fell smoothly to 10.5μ and the film was essentially opaque beyond that to 16μ. The material lost about 4% in weight when ignited to 1200°C. The material is thus a slightly hygroscopic, slightly porous, amorphous, essentially unhydrated alumina.

Experiments are in progress to determine the transient or metastable transition phases which might be formed during the course of its thermal transformation to α-alumina. Differential thermal analysis showed transformation beginning at about 760°C, with a double peak at about 820°C and 860°C. Delta-alumina has been identified by X-ray diffraction as one intermediate phase. It appears on heating to 700°C or 900°C for 1/2 hour and is unchanged on subsequent heatings at these temperatures for up to 32 hours. There is some possibility that one or more less-ordered transition phases may be formed and a search for these is continuing.

REFERENCES

[1] L. Brewer and A. W. Searcy. J. Am. Chem. Soc. 73, 5308 (1951).

[2] G. W. Sears and L. Navias. J. Chem. Phys. 30, 1111 (1959).

[3] J. Drowart, G. DeMaria, R. P. Burns, and M. G. Inghram. J. Chem. Phys. 32, 1366 (1960).

[4] R. F. Hampson and R. F. Walker. J. Res. Nat. Bur. Stand. 65A, 289 (1961).

[5] J. J. Diamond. J. Am. Ceram. Soc. 43, 1 (1960).

Chapter B-5

ALLOYS AND INTERSTITIAL COMPOUNDS OF THE LIGHT METALS AND THE LIGHT METALS WITH TUNGSTEN

by Thomas W. Mears

Aluminum-Zirconium System

Three papers relating to this system were found in Current Chemical Titles [1,2,3], but only one [3] was available for abstracting.

Edshammer [3] has reviewed the structural data on the aluminum-zirconium alloys and attempted to correlate the several structures. His summary of the data is given below:

Compound	Structure Type	Lattice Constants (A) a	b	c	Reference
Zr_3Al	$L1_2$	4.372			[4]
Zr_2Al	$D8_2$	4.894		5.928	[5] [6]
Zr_5Al_3	D8m	11.049		5.396	[7]
Zr_3Al_2	Tetragonal	7.630		6.998	[8]
Zr_4Al_3	Hexagonal	5.433		5.390	[9]
Zr_2Al_3	Orthorhombic	9.601	13.906	5.57	[6] [10]
$ZrAl_2$	C14	5.282		8.748	[11]
$ZrAl_3$	DO_{23}	4.306		16.90	[12]

Aluminum-Tungsten System

The phase diagram for the aluminium-tungsten system is given by Clark [13] and is reproduced in Hansen's book [14]. The existence of the phases WAl_7, WAl_5, WAl_4, WAl_3, and WAl_2 is suggested, but not confirmed [15,16,17]. However, the forms containing between 0 and 20 atomic percent tungsten are well established, namely WAl_{12}, WAl_5, and WAl_4. There is some indication of the existence of another phase by reaction of aluminum with WAl_{12} below 580°C.

WAl_{12} has a body-centered structure with a = 7.580 A, and with two WAl_{12} units per cell [18].

Beryllium-Tungsten System

Three intermetallic compounds of beryllium and tungsten have been reported [19].

Be_2W has an hexagonal $MgZn_2$ (C14) structure, a=4.446A, c=7.289A, c/a=1.639.

$Be_{13}W$ has a tetragonal lattice, a=10.14A, c=4.23A, c/a=0.416. The structure was chosen because of the analogy to $Be_{13}Mo$.

$Be_{12}W$ has lattice constants a=7.220 ±0.004, c=4.224 ±0.004 Kx [20].

An unidentified low-melting alloy was formed by deposition of beryllium on a tungsten filament at 1230°C [21].

An alloy of 1 wt. percent tungsten, cooled from the melt, gave a two-phase eutectic [22].

Magnesium-Tungsten System

Tungsten does not affect the lattice of magnesium nor does it form alloys or intermetallic compounds [23,24,25].

Tungsten-Zirconium System

Hansen [14] gives a phase diagram based on two independent sources [26,27]. This diagram shows the following:

1. A eutectoid at 860°C (0.25 at. % W) (α-and β-Zr forms)
2. A eutectic at 1660°C (10 at. % W)
3. A peritectic melt at 2150°C (33 at. %). Solubility of tungsten in zirconium, 6 atomic percent. Solubility of tungsten in α-zirconium less than 0.25 atomic percent.

ZrW_2 has a cubic $MgCo_2$ (C15) type structure with a=7.631 [28] or 7.615A [29].

References

1. A. J. Goldak, Trans. Met. Soc. AIME 221, 639 (1961).

2. H. Nowotny, O. Schob, and F. Benesovsky, Monatsch 92, 1300 (1961).

3. L. E. Edshammer, Acta Chem. Scand. 16, 20 (1962).

4. J. H. Keeler and J. H. Mallory, J. Metals 7, 394 (1955).

5. C. G. Wilson and D. Sams, Acta Cryst. 14, 71 (1961).

6. K. Schubert, T. R. Arantharaman, H. O. K. Ata, H. G. Meissner, M. Potschke, W. Rossteutscher and E. Stoltz, Naturwiss. 47, 512 (1960).

7. L. E. Edshammer and S. Anderson, Acta Chem. Scand. 14, 223 (1960).

8. C. G. Wilson and F. J. Spooner, Acta Cryst. 13, 358 (1960).

9. C. G. Wilson, D. K. Thomas and F. J. Spooner, Acta Cryst. 13, 56 (1960).

10. T. J. Renouf and C. A. Bevers, Acta Cryst. 14, 469 (1961).

11. C. G. Wilson, Acta Cryst. 12, 660 (1959).

12. G. Brauer, Z. anorg Chem. 242, 1 (1939).

13. W. J. Clark, J. Inst. Metals 66, 271-286 (1940).

14. M. Hansen, Constitution of Binary Alloys, McGraw-Hill Publishing Company (1958).

15. J. Matthews and W. Campbell, J. Am. Chem. Soc. 24, 256 (1902).

16. F. Wöhler and F. Michel, Ann. 115, 103 (1860).

17. L. Guillet, Compt. rend. 132, 1112 (1901).

18. J. Adam and J. B. Rich, Acta Cryst. 7, 810 (1954).

19. L. Misch, Metallwirtschaft 15, 163 (1936).

20. E. I. Gladyshevskii and P. I. Kripyakevich, Kristallografiya 2, 742 (1957).

21. L. Hackspill and J. Besson, Bull. soc. chim. France 16, 113 (1949).

22. A. R. Kaufman, P. Gordon and D. W. Lillie, Trans. ASM 42, 801 (1950).

23. R. S. Bush, Trans. AIME 188, 1460 (1950).

24. D. Kramer, Abhand. Inst. Metallkutt u. Electromet. Tech. Hochsch., Aachen 1, 8 (1916).

25. F. Sauerwald, Z. anorg. Chem. 258, 296 (1949).

26. R. F. Domagola, D. J. McPherson and M. Hansen, Trans AIME 197, 73 (1953).

27. G. A. Grach and G. F. Slattery, Trans. AIME 197, 747 (1953).

28. A. Claasen and W. G. Burgers, Z. Krist A86, 100 (1933).

29. R. P. Elliott, Armour Research Foundation Tech. Rept. 1, OSR Technical Note OSR-TN-247 (1954).

Chapter B-6

RECENT ADDITIONS TO THE LITERATURE RELATED TO THE HEATS OF FORMATION OF COMPOUNDS OF SELECTED ELEMENTS

by M. C. Bracken and G. T. Armstrong

The following articles, classified by element have been selected from the literature since the last listing of new literature (NBS Report No. 7437, January, 1962). Cross references under an element heading indicate that a compound containing the element was referred to in a paper, to be found classified under element.

A. Aluminum Compounds

1. Thermochemistry of alloys. C.A.56, 8080d (1962). A. Schneider, H. Klotz, J. Stendel, and G. Strauss, Pure Appl. Chem. 2, 13-16 (1961).

   ΔF_f is reported for $A\ell_2Zr$, $A\ell_3Zr_2$, $A\ell_3Zr_4$.

2. Estimation of the heats of formation of gaseous combustion product molecules. C.A.56, 8081f (1962). C. J. O'Brien, J. R. Perrin and J. Perrine, pp 5-17, Kinetics, Equilibria and Performance of High Temperature Systems, Proc. 1st Conf., Los Angeles, Calif., 1959, G. S. Bahn and E. E. Zukoski, Eds. (Butterworths, Washington 14, D. C., 1960).

   Compounds of elements in Periods 1, 2 and 3, and K and Br are included in the correlations.

3. Heats of formation of cryolite and the aluminum fluorides. C.A.56, 8419g (1962). P. Gross, C. Haymen and D. I. Levi, Met. Soc. Conf. 8, 903-8 (1961). A better reference is: International Symposium on the Physical Chemistry of Process Metallurgy, Pittsburgh, 1959. Physical Chemistry of Process Metallurgy, G. R. St. Pierre, Editor, (Interscience Publishers, New York, 1961).

   $A\ell F$, $A\ell F_3$, NaF, $Na_3A\ell F_6$, PbF_2 heats of formation are given. This work, previously referred to, has finally been published.

4. Thermodynamics of the compounds formed by tantalum, niobium, titanium, zirconium, hafnium and aluminum chlorides with alkali metal chlorides. C.A.56, 4163b (1962). I. S. Morozov and D. Ya. Toptygin, Izvest. Akad. Nauk S.S.S.R., Otdel. Khim. Nauk 1959, 1920-70.

   ΔH, ΔS and ΔF are given for the dissociation of these double salts.

5. The heats of solution in liquid tin of the Group III elements aluminum, gallium, indium and thallium. C.A.56, 4166a (1962). J. B. Cohen, B. W. Howlett and M. B. Bever, Trans. AIME 221, 683-6 (1961).

6. Thermodynamic considerations in the aluminum producing electrolyte. C.A.56, 4167i (1962). W. B. Frank, J. Phys. Chem. 65, 2081-7 (1961).

   $A\ell F_3$, NaF, $NaA\ell F_4$, $Na_3A\ell F_6$, $NaA\ell O_2$, $A\ell_2O_3$. Equilibria at 1300°K and thermodynamic values are discussed.

7. Relation between chemical heats of hydration of ions and their coefficients of polarization. C.A.56, 8081g (1962). D. Gerdzhikov, Compt. Rend. Acad. Bulgare Sci. 14, 471-3 (1961) (in French).

   $A\ell$, Be, Mg, Li, Na, F, $C\ell$ and other ions.

8. Chemical species in high temperature systems. C.A.56, 8081e (1962). R. S. Scheffee and C. B. Henderson, pp 1-4. Kinetics, Equilibria and Performance of High Temperature Systems, Proc. 1st Conf., Los Angeles, Calif., 1959, G. S. Bahn and E. E. Zukoski, Eds. (Butterworths, Washington 14, D.C., 1960).

   Heats of formation of metal subhalides, mixed halides, oxyhalides, hydroxides are estimated or discussed.

9. Free energies of formation of gaseous metal oxides. C.A.56, 11001h (1962). M. Gleiser, Trans. AIME 221, 300-4 (1961).

   Charts are given for estimating free energy changes involving vaporization of oxides of $A\ell$, B, Be, W, Zr, and other metals.

10. Results and problems of compounds of the system oxide-water. C.A.56, 5443e (1962). O. Glemser, Angew. Chem. 73, 785-805 (1961).

    Reviews vaporization of Li, Na and other alkali hydroxides, BeO, WO_3 and other oxides in the presence of water, $B(OH)_3$, BOOH, the system $A\ell_2O_3$-H_2O, $CO(OH)_2$, NO_2OH, NOOH, $C\ell OH$, $C\ell O_3OH$ and other compounds.

11. Aluminum binary equilibrium diagrams. E. H. Wright and L. A. Willey, Aluminum Company of America, Technical Paper No. 15, Pittsburgh, Pennsylvania, 1960.

    Phase diagrams for $A\ell$-B, $A\ell$-Be, $A\ell$-C, $A\ell$-Hg, $A\ell$-Li, $A\ell$-Mg, $A\ell$-Na, $A\ell$-Pb, $A\ell$-Ti, $A\ell$-W, $A\ell$-Zr.

12. Alumina properties. J. W. Newsome, H. W. Heiser, A. S. Russell, and H. C. Stumpf. Aluminum Company of America Technical Paper No. 10 (2nd Revision), Pittsburgh, Pennsylvania, 1960.

    Al_2O_3, $Al_2O_3 \cdot H_2O$, $Al_2O_3 \cdot 3H_2O$ in various phases are reviewed.

13. Estimation of the heats of formation of gaseous combustion product molecules. C.A.56, 8081b (1962). R. R. Koppang, C. M. Sherwood, G. S. Bahn, pp 18-29. Kinetics, Equilibria and Performance of High Temperature Systems, Proc. 1st Conf., Los Angeles, Calif., 1959. G. S. Bahn and E. E. Zukoski, Eds. (Butterworths, Washington 14, D. C., 1960).

    New tables are presented.

14. See also K-4.

B. Boron

1. Nitrogen Reaction in Explosives. C.A.52, 21108h (1958). A. Ya. Apin, U. A. Lebedev, and O. E. Nefedeva, Zhur. Fiz. Khim. 32, No. 4, 819 (1958).

    BN, PbN_6. ΔHf is given for BN.

2. Heats of formation of borides of some transition metals. C.A.51, 6310c (1957). G. V. Samsonov, Zhur. Fiz. Khim. 30, 2057 (1956).

    TiB_2, ZrB_2, W_2B_5. ΔHf.

3. Mass spectrometric study of the vaporization of the Ti-B system. P. O. Schissel and O. C. Trulson, Union Carbide Corp. Report URS-60, February 1962.

    Vaporization study of Ti-B system.

4. High temperature evaporation and thermodynamic properties of zirconium diboride. J. M. Leitnaker, M. G. Bowman and P. W. Gilles, J. Chem. Phys. 36, 350 (1962).

    The heat of vaporization of ZrB_2 was determined.

5. Thermodynamic and kinetic studies for a refractory materials program. Second semi-annual progress report, 1 January to 30 June 1961. A.D. WADD Contract AF 33(616)-7472 Task 7472, A. D. Little, Inc., San Francisco, Calif. pp 21-24. John L. Margrave, contributing author.

    Enthalpy and entropy of ZrB_2 to 1200°K.

6. Molecular potentials, constants and thermodynamic functions of the boron halides. C.A.56, 10926g (1962). J. Jakes and D. Papousek, Collection Czech. Chem. Commun. 26, 2110-23 (1961).

7. Thermal functions and heats of formation of some of the vapor species in the boron-oxygen-hydrogen system at elevated temperatures. C.A.56, 10998b (1962). D. White, P. N. Walsh, D. E. Mann, and A. Sommer. U. S. Dept. Comm., Office Tech. Serv., P.B. Report 147,086, 22 pp (1959).

B_2O_3, B_2O_2, HBO_2, $(HBO_2)_2$.

8. Heats of formation of some inorganic compounds by fluorine bomb calorimetry. C.A.56, 10998 (1962). S. S. Wise, U. S. At. Energy Comm. ANL-6472, 71 pp (1962).

ΔHf of BF_3, BN.

9. Determination of the differences in vapor pressures of $B^{10}F_3$ and $B^{11}F_3$. C.A.56, 8026g (1962). A. V. Borison and I. G. Gverdtsiteli, Zhur. Fiz. Khim. 35, 1212-14 (1961).

10. The heats of decomposition of some higher boron hydrides. C.A.56, 6725b (1962). S. R. Gunn and L. G. Green, J. Phys. Chem. 65, 2173-5 (1961).

Study includes B_4H_{10}, B_5H_9, B_5H_{11} and B_6H_{10}.

11. The standard heat of formation of α- and β-modifications of metaboric acid. C.A.56, 1004e (1962). N. D. Sokolova, S. M. Skuratov, A. M. Shemonaeva, and V. M. Yuldasheva, Zhur. Neorg. Khim. 6, 774-6 (1961).

12. Determination of the heat of sublimation of boron by the mass spectrometric method. C.A.56, 1005g (1962). P. A. Akishin, O. T. Nikitin and L. N. Gorokhov, Doklady Akad. Nauk S.S.S.R. 129, 1075-8 (1959).

$\Delta H^{\circ}_{0} = 131.6 \pm 5$ kcal (g atom)$^{-1}$.

13. Thermodynamic properties and characteristics of boron nitride at high temperatures. C.A.56, 10997h (1962). V. V. Fesenko, Poroshkovaya. Met. Akad. Nauk Ukr. S.S.R. 1, No. 4, 80-5 (1961).

A vaporization study of BN.

14. Chemical properties of hexaborides of alkaline earth metals. C.A.56, 9680b (1962). N. V. Vekshina and L. Ya. Markovskii, Zhur. Priklad. Khim. 34, 2171-5 (1961).

    The stabilities of TiB_2 and ZrB_2 at high temperatures are discussed.

15. See also A-2, A-8, A-9, A-11, A-13, M-1, R-1.

C. Beryllium

1. Energies of the gaseous alkaline earth halides. C.A.56, 2047i (1962). D. C. Cubicciotti, Jr., J. Phys. Chem. 65, 1058-9 (1961).

   The study includes BeF_2, $BeC\ell_2$, MgF_2, $MgC\ell_2$ and others.

2. Enthalpy of beryllium and lithium oxides at high temperatures. C.A.56, 70c (1962). E. N. Rodigina and K. Z. Gomel'skii, Zhur. Fiz. Khim. 35, 1828-31 (1961).

3. See also A-2, A-7, A-8, A-9, A-10, A-11, A-13, K-5.

D. Bromine

1. Heats of formation of bromine fluorides. C.A.56, 9506g (1962). L. Stein, J. Phys. Chem. 66, 288-9 (1962).

   From equilibrium measurements the heats of formation of BrF, BrF_3 and BrF_5 are calculated.

2. Moving bomb method for combustion calorimetry of organic bromine compounds. C.A.56, 8514b (1962). L. Bjellerup, Acta. Chem. Scand. 13, 1511-41 (1959).

3. Combustion calorimetry of organic bromine compounds: the accuracy of data obtained with a moving bomb technique. C.A.56, 6723h (1962). L. Bjellerup, Pure Appl. Chem. 2, 45-7 (1961).

4. Reduction to standard heat of combustion of bomb calorimetric data for organic bromine compounds. C.A.56, 6725c (1962). L. Bjellerup, Acta Chem. Scand. 14, 617-24 (1960).

5. Heat of formation of the hypobromite ion. C.A.56, 4163h (1962). J. E. McDonald and J. W. Cobble, J. Phys. Chem. 65, 2014-15 (1961).

6. See also A-2, A-7, A-8, A-13, B-6, I-1, K-5, K-6, K-8, K-9, K-12, L-3, N-1, N-3, N-5, O-2, Q-1, Q-2, S-2.

E. Carbon

1. The equilibrium composition of the carbon-hydrogen system at elevated temperatures. C.A.56, 41621 (1962). R. E. Duff and S. H. Bauer, U. S. At. Energy Comm. LA-2556, 177 pp (1961).

2. Thermodynamic functions of the gaseous dioxides of carbon, nitrogen, sulfur, and chlorine, and of carbon disulfide and oxysulfide. C.A.56, 2953a (1962). J. S. Gordon, J. Chem. Eng. Data 6, 390-4 (1961).

3. Heat of sublimation and dissociation energy of gaseous C_2. L. Brewer, W. T. Hicks, and O. H. Krikorian, J. Chem. Phys. 36, 182-8 (1962).

4. Dissociation energy of cyanogen and related quantities by x-ray densitometry of shock waves. C.A.56, 2008f (1962). H. T. Knight and J. P. Rink, J. Chem. Phys. 35, 199-208 (1961).

   C_2N_2 and HCN were studied.

5. Equilibria at high temperatures for the formation of the molecular species C_2, C_3, Cu_2 and Si_2. S. Zaff, L. E. Ashley, and C. M. Cobb, Paper No. 8, Kinetics, Equilibria and Performance of High Temperature Systems. Proc. 1st Conf., Los Angeles, Calif., 1959. G. S. Bahn and E. E. Zukoski, Eds. (Butterworths, Washington 14, D.C., 1960).

6. See also A-2, A-10, A-11, A-13, S-1.

F. Chlorine

1. Integral heats of solution in water at 25° of perchloric anhydride and its mixtures with perchloric acid. C.A.56, 73i (1962). V. Ya. Rosolovskii, N. V. Krivtsov and A. A. Zinov'ev, Zhur. Neorg. Khim. 5, 778-81 (1960).

2. An approximate method for calculating the heats of formation of inorganic compounds. C.A.56, 73h (1962). L. A. Reznitskii, Zhur. Fiz. Khim. 35, 1852-9 (1961); also Russian J. Phys. Chem. 35, 912-5 (1961).

   F^-, Cl^-, O^{-2}, O_2^{-2}, OH^-, H^-, ClO_3^-, WO_4^{-2}, NO_3^-, NO_2^- and other anions are considered.

3. Integral heats of solution of perchloric acid. C.A.56, 74d (1962). N. V. Krivtsov, V. Ya. Rosolovskii, and A. A. Zinov'ev, Zhur. Neorg. Khim. 5, 772-4 (1960).

   Heats of solution of $HC\ell O_4$, $HC\ell O_4 \cdot H_2O$ and $HC\ell O_4 \cdot 2H_2O$ were measured.

4. See also A-2, A-4, A-7, A-8, A-13, B-6, C-1, E-2, I-1, K-2, K-5, K-8, K-9, K-10, K-12, L-1, L-3, N-1, N-4, N-5, O-2, P-1, Q-1, Q-2, S-2, S-3.

G. Fluorine

1. Fluorine bomb calorimetry. C.A.56, 6722i (1962). W. N. Hubbard, J. L. Settle, and H. M. Feder, Pure Appl. Chem. 2, 39-44 (1961).

2. Thermochemistry of organic fluorine compounds and carbon compounds of metals by rotating bomb calorimetry. C.A.56, 2954c (1962). W. D. Good and D. W. Scott, Pure Appl. Chem. 2, 77-82 (1961).

3. Tetrafluorohydrazine-difluoroamino radical equilibrium. C.A.56, 1010f (1962). F. A. Johnson and C. B. Colburn, J. Am. Chem. Soc. 83, 3043-7 (1961).

4. Mass spectrometric study of the thermal dissociation of N_2F_4. C.A.56, 9696d (1962). J. T. Herron and V. H. Dibeler, J. Chem. Phys. 35, 747-8 (1961).

5. See also A-2, A-3, A-6, A-7, A-8, A-13, B-6, B-8, B-9, C-1, F-2, K-1, K-2, K-3, K-5, K-8, K-9, K-12, L-3, N-2, N-6, O-2, Q-1.

H. Hydrogen

1. See References A-2, A-8, A-10, A-12, A-13, B-7, B-11, E-1, E-4, F-2, F-3, K-3, K-6, K-7, K-8, K-10, K-11, K-13, L-3, L-4, M-1, O-1, O-2, P-1, Q-3, S-2, S-3.

I. Mercury

1. Enthalpies and entropies of formation of Hg(II) halide 1:1 complex ions. C.A.56, 4169b (1962).

   $HgC\ell^+$, $HgC\ell_2$, $HgBr^+$, $HgBr_2$, HgI^+, HgI_2.

2. Physical properties of mercuric oxide. C.A.56, 2007e (1962). P. Laruelle, Ann. Chim. (Paris) 5, 1315-72 (1960).

   A review with 67 references.

3. See also A-11.

J. Iodine

1. Determination of dissociation constants and heats of formation of molecules by flame photometry. VII. Flame photometer study of the IO radical. C.A.56, 73d (1962). L. F. Phillips and T. M. Sugden, Trans. Faraday Soc. 57, 914-20 (1961).

2. See also I-1, K-5, K-9, O-2, Q-1, S-2.

K. Lithium

1. Melting points of inorganic fluorides. C.A.56, 10935d (1962). B. Porter and E. A. Brown, J. Am. Chem. Soc. 45, 49 (1962).

   LiF, 846°; NaF, 994°.

2. The thermodynamic properties of the alkali halides. C.A.56, 10997g (1962). L. Brewer, U. S. At. Energy Comm. UCRL-9952, 7 pp (1961).

   LiF, LiCℓ, NaF, NaCℓ.

3. Heat capacities of lithium and sodium monohydrogen difluorides from 6 to 305°K. C.A.56, 4170a (1962). E. F. Westrum, Jr., and G. A. Burney, J. Phys. Chem. 65, 344-8 (1961).

   $LiHF_2$, $NaHF_2$. The dissociation pressure of $LiHF_2$ was measured and the free energy of formation is reported.

4. Thermodynamics of the vacuo-thermal preparation of lithium. C.A.56, 2952g (1962). F. I. Shamrai and T. F. Fedorov, Redkie Shchelochnye Elementy, Akad. Nauk S.S.S.R., Sibir. Otdel. Sbornik Dokladov Soveshchaniya 1958, 25-9.

   Equilibrium studies involving Li, Li_2O, $Aℓ_2O_3$, $Li_2O \cdot Aℓ_2O_3$, O_2 and other compounds.

5. Law of corresponding states for fused salts. C.A.56, 951h (1962). H. Reiss, S. W. Mayer, and J. Katz, U. S. At. Energy Comm. NAA-SR-6131, 18 pp (1961); J. Chem. Phys. 35, 820-6 (1961).

   Group I and II oxides and halides are correlated.

6. Thermodynamic properties and thermal diagrams of the binary system lithium bromide-water. C.A.56, 1005h (1962). H. Loewer, Kaeltechnik 13, 178-84 (1961).

   Vapor pressure, heats of solution and dilution, entropy and enthalpy are reviewed.

7. Thermodynamic studies at low temperatures. XI. Heat capacity of lithium hydride between 3.7 and 295°K and the entropy and enthalpy at 298.15°K. C.A.56, 71b (1962). V. N. Kostryukov, Zhur. Fiz. Khim. 35, 1759-62 (1961).

8. "Mendeleev's rule" and its utilization in the calculations of physicochemical magnitudes. I. Heats of formation. C.A.56, 72f (1962). B. F. Yudin, Trudy Gosudarst. Inst. Priklad. Khim. 1960, No. 46, 102-14.

   Calculations and correlations include LiOH, Li_2O_2, LiF, NaOH, Na_2O_2, NaF, NaCℓ, NaBr and other compounds.

9. Determination of dissociation constants and heats of formation of molecules by flame photometry. VIII. Stabilities of the gaseous diatomic halides of certain metals. C.A.56, 73e (1962). E. M. Bulewicz, L. F. Phillips, and T. M. Sugden, Trans. Faraday Soc. 57, 921-31 (1961).

   Li, Na and other metal halides were studied.

10. Application of Berthelot's principle in calculating standard entropies of inorganic solids. C.A.56, 76g (1962). N. N. Drozin, Zhur. Fiz. Khim. 35, 1789-93 (1961).

    Values were calculated and compared with experimental values for LiCℓ, LiOH, NaCℓ, $NaC\ell O_3$, NaOH and other compounds.

11. Heats of formation of certain double compounds. C.A.56, 9505i (1962). N. A. Reshetkinov, Zhur. Neorg. Khim. 6, 682-6 (1961).

    Heats of solution of LiOH and NaOH were determined.

12. "Mendeleev's rule" and its utilization in calculations of physicochemical magnitudes. II. Entropy, heat capacity, temperature and heat of phase transition, and sequence in the periodic table. C.A.56, 72g (1962). B. F. Yudin, Trudy Gosudarst. Inst. Priklad. Khim. 1960, No. 46, 115-25.

    Correlations include Li, Na, F, Cℓ, Br, N and other elements in various combinations.

13. Binding energy of LiH. C.A.56, 9583h (1962). B. Musulin and D. R. Jamieson, Trans. Illinois State Acad. Sci. 51, 51-4 (1958).

14. See also A-2, A-4, A-7, A-8, A-10, A-11, A-13, C-1.

L. Magnesium

1. Metal-molten salt solutions. Phase equilibrium in the systems Mg plus $MgC\ell_2$ and Ca plus CaF_2. C.A.56, 10994g (1962). P. S. Rogers, J. W. Tomlinson, and F. D. Richardson, Met. Soc. Conf. 8, 909-24 (1961).

2. Approximate calculations of the thermodynamic characteristics of the tungstates and molybdates of bivalent metals. C.A.56, 4163c (1962). L.A. Zharkova and Ya. I. Gerasimov, Zhur. Fiz. Khim. 35, 2291-6 (1961).

   ΔH^{o}_{298} is calculated for $MgWO_4$, $PbWO_4$, and other compounds.

3. Thermodynamics of unitype chemical reactions and unitype compounds. C.A.56, 1007h (1962). V. A. Kireev, Zhur. Fiz. Khim. 35, 1393-1405 (1961).

   Estimates are made of ΔHf, ΔFf and ΔSf for $MgTiO_3$, HF, $HC\ell$, HBr and other compounds and the values are correlated.

4. The thermodynamics of the conversion of magnesium and manganese oxides to sulfides. C.A.56, 245a (1962). E. W. Dewing, J. Iron Steel Inst. (London) 195, 56-8 (1960).

   Equilibria in the reaction: $MgS + H_2O = MgO + H_2S$ were studied by a gas circulation method.

5. See also A-2, A-7, A-8, A-11, A-13, C-1, K-5.

M. Nitrogen

1. Far infrared spectra. C.A.56, 9589h (1962). R. C. Lord, U. S. Dept. Comm. Office Tech. Serv., PB Rept. 161, 738, 29 pp (1960).

   Thermodynamic functions are given for N_2H_4, B_2H_6 and other compounds.

2. Evaporation equilibriums in the system nitrogen-oxygen at 77.50°K. C.A.56, 63b (1962). G. Wilhelm and G. Schneider, Z. physik. Chem. 29, 43-6 (1961).

3. Thermodynamic properties of mixtures at low temperatures. C.A. 56, 9505f (1962). J. J. M. Beenakker, H. F. P. Knaap, and C. M. Knobler, Proc. Intern. Conf. Low Temp. Phys., 7th, Toronto, Can., 1960, 707-9 (Pub. 1961).

   Heat of mixing liquid N_2 and O_2.

4. Thermodynamic properties of some oxides of nitrogen. C.A. 56, 8079f (1962). I. C. Hisatsune, J. Phys. Chem. 65, 2249-53 (1961).

   C_p^o, S^o, ΔHf^o, ΔFf^o were calculated for N_2O_3, N_2O_4, N_2O_5 and NO_3.

5. Heat of dissociation of nitrogen. C.A. 56, 6724g (1962). G. Glockler, Pure Appl. Chem. 2, 49-53 (1961).

   Discussion based on internuclear distance.

6. See also A-2, A-10, A-13, B-1, B-8, B-13, E-2, E-4, F-2, G-4, K-12, O-2, P-1.

N. Sodium

1. Low range vapor pressures of alkali chlorides and bromides. C.A. 56, 10929i (1962). E. M. Braun, Ind. Chemist 38, 62 (1962). A nomograph for NaCℓ, NaBr and other compounds.
2. Freezing point depressions in sodium fluoride. Effect of alkaline earth fluorides. C.A. 56, 8079a (1962). S. Cantor, J. Phys. Chem. 65, 2208-10 (1961).

3. Thermodynamic properties of molten salt solutions in the system $PbBr_2$-NaBr. C.A. 56, 4162h (1962). M. F. Lantratov, T. N. Shevlyakova, Zhur. Neorg. Khim. 6, 192-8 (1961). From e.m.f. measurements activities and other properties were calculated.
4. The thermodynamic properties of high-temperature aqueous solutions. I. Standard partial molal heat capacities of sodium chloride and barium chloride from 0° to 100°. C.A. 56, 2956b (1962). C. M. Criss and J. W. Cobble, J. Am. Chem. Soc. 83, 3223-8 (1961).

   The heat of solution of NaCℓ was measured.

5. Molecular association in alkali halide vapors. C.A. 56, 944i (1962). S. Datz, W. T. Smith, Jr., and E. H. Taylor, J. Chem. Phys. 34, 558-64 (1961).

   Studies included NaCℓ, $Na_2Cℓ_2$, NaBr, Na_2Br_2 and other compounds.

6. Intercrystalline energies in the alkali halides. C.A.56, 9530b (1962). D. P. Spitzer, J. Phys. Chem. 66, 31-8 (1962).

   NaF grain boundary energy was calculated from measured interfacial properties.

7. See also A-2, A-3, A-4, A-6, A-7, A-8, A-10, A-11, A-13, K-1, K-2, K-3, K-5, K-8, K-9, K-10, K-11, K-12.

O. Oxygen

1. The thermodynamic properties of the products of H_2-O_2 combustion at elevated temperatures. C.A.56, 8081a (1962). W. A. Moffatt, F. D. Skinner, and R. J. Zaworski, pp 53-7. Kinetics, Equilibria and Performance of High Temperature Systems, Proc. 1st Conf., Los Angeles, Calif., 1959. G. S. Bahn and E. E. Zukoski, Eds. (Butterworths, Washington 14, D. C., 1960).

   O, O_2, OH, H_2O are treated.

2. On the apparent divergence of the thermodynamic properties of dilute gases at high temperatures: thermodynamic functions for diatomic molecules. C.A.56, 8081d(1962). L. Haar, pp 35-8. Ibid.

3. See also A-2, A-6, A-8, A-9, A-10, A-12, A-13, B-7, B-11, E-2, F-2, F-3, I-2, J-1, K-4, K-5, K-6, K-8, K-10, K-11, L-2, L-3, L-4, M-2, M-3, M-4, P-2, S-2, S-3.

P. Lead

1. Thermographic method for measurement of saturation vapor pressure of difficultly volatile substances. C.A.56, 2900d (1962). G. I. Novikov and O. G. Polyachenok, Zhur. Neorg. Khim. 6, 1951-2 (1961).

   Vapor pressures of $PbC\ell_2$ and $NH_4C\ell$ are presented.

2. Enthalpy and specific heat of yellow lead monoxide at high temperatures. C.A.56, 76e (1962). E. N. Radigina, K. Z. Gomel'skii, and V. F. Luginina, Zhur. Fiz. Khim. 35, 1799-1802 (1961).

   The heat of fusion is given for PbO.

3. See also A-3, A-11, B-1, L-2, N-3.

Q. Titanium

1. Halides of the transition elements of the first long period. C.A.56, 5460f (1962). M. Barber, J. W. Linnett, and N. H. Taylor, J. Chem. Soc. (London) 1961, 3323-32.

   Stabilities are calculated for crystalline TiX, TiX_2, TiX_3, where X is F, Cℓ, Br, I, and the halides of other metals, and compared with experiment.

2. Some thermodynamic values for four titanium halides. C.A.56, 4164e (1962). E. G. King, W. W. Weller, A. U. Christensen, and K. K. Kelley. U. S. Bur. Mines, Rept. Invest. No. 5799 (1961).

   ΔHf and ΔFf are given as functions of temperature for $TiC\ell_3$, $TiBr_3$ and $TiBr_4$.

3. Heat capacity and thermodynamic functions of TiH_2 in the range 24 to 363°K. C.A.56, 4167f (1962). B. Stalinski and Z. Bregonski, Bull. Acad. Polon. Sci., Ser. Sci. Chim. 8, 243-8 (1960).

   ΔHf and ΔSf are given.

4. See also A-4, A-11, B-2, B-3, B-14, L-3.

R. Tungsten

1. Reactions in the ternary zirconium-tungsten-boron; phase domains, comparison between results obtained and predictions. C.A.56, 11327g (1962). A. Chretien and J. Helgorsky, Compt. Rend. 253, 2693-5 (1961).

   Phases found were ZrB_2, ZrW_2, W_2B, WB, W_2B_5, WB_4. Results were in agreement with thermodynamic predictions.

2. See also A-9, A-10, A-11, B-2, F-2, L-2.

S. Zirconium

1. The vaporization behaviour and thermodynamic stability of zirconium carbide at high temperature. C.A.56, 5458i (1962). B. D. Pollack, U. S. At. Energy Comm. NAA-SR-5439, 15 pp (1961).

2. Thermochemistry of zirconium halides. C.A. 56, 4164f (1962). A. G. Turnbull, J. Chem. Phys. 65, 1652-4 (1961).

   Heats of formation are given for $ZrBr_4$, ZrI_4, ZrO_2, $ZrO(OH)^+(aq)$. Heat of hydrolysis of $ZrC\ell_4$ was measured.

3. On zirconium tetrafluoride hydrate, zirconium hydroxofluorides and their condensation products. L. Kolditz and A. Feltz, Z. anorg. u. allgem. Chem. 310, 217-224 (1961).

   Thermal decomposition of $ZrF_4 \cdot H_2O$ is described. Nine compounds with Zr, F, O and H in various proportions are listed.

4. See also A-1, A-4, A-9, A-11, B-2, B-4, B-5, B-14, R-1.

Chapter B-7

LITERATURE SURVEY AND ANALYSIS OF HEAT-CAPACITY DATA OF SOME SELECTED COMPOUNDS CONTAINING Li, Mg, Aℓ, Si, Ti, W, and Pb

by George T. Furukawa and Martin L. Reilly

The work given in this chapter is a continuation of systematic survey of literature data on heat capcity to complement the experimental low-temperature heat-capacity measurements being made. The present report gives results of the analysis of low and high temperature heat data for some selected compounds containing Li, Mg, Aℓ, Si, Ti, W, and Pb. As in the past reports issued on this work, the original experimental data were examined wherever feasible and comparisons made with existing compilations of thermodynamic functions. In the analysis of low-temperature data the original values of heat capacity given in the papers were used. These values were joined smoothly to the values of heat capacity derived from the high-temperature enthalpy equations given relative to 298°K. In most of the cases the enthalpy equations given in the original papers were used. Others were taken from the Bureau of Mines Bulletin 584 [32]. In the case of tungsten the enthalpy equation was obtained by fitting selected experimental data by the method of least squares. Most of the substances described in this report were investigated at the Bureau of Mines Laboratories in Berkeley, California. Therefore, the enthalpy equation selected from the original papers are the same in most cases as those given in the Bureau of Mines Bulletin 584 [32]. In smoothly joining the low-temperature data to the high-temperature enthalpy data through the enthalpy equation, an effort was made not to change the enthalpy increment given by the equation in the interval 298.15° to 400°K, where small adjustments in the heat capacity were made. Values of the enthalpy increment obtained for this temperature interval are compared in this report with values considered representative of experiment and with values calculated from the original enthalpy equation. Values of thermodynamic functions above about 400°K are based entirely on the enthalpy equations. Some reasonable extrapolation above the experimental temperature range was made. In most of the cases the enthalpy equations given by the various investigators were found to give considerably higher enthalpy increments than the experimental value in the interval 298.15° to 400°K.

Low-temperature heat-capacity measurements reported by the Bureau of Mines Laboratories in Berkeley, cover the range 53° to about room temperature. Debye-Einstein heat-capacity equations fitted to the experimental data are used by the above laboratory to extrapolate below the experimental temperature range. These equations were used in this report to obtain values of heat capacity in the range 0° to about 53°K whenever additional experimental data were lacking at the lower temperatures.

The thermodynamic functions were calculated by numerical integration of smoothed values of heat capacity. Smoothed values of the low-temperature measurements were obtained from the experimental data by a method of successive approximation using a smoothing curve. These values were joined smoothly with adjustments to values calculated from the Debye-Einstein heat-capacity equations and to values derived from the enthalpy equations where applicable. The smoothing and integration were performed on an IBM 7090 computer at the National Bureau of Standards.

The substances are discussed separately with references to the experimental data that were examined. Values of S°_{298} obtained are summarized and compared in a table at the end of the discussion. The atomic weights were taken from the 1961 atomic weights based on C-12 [21].

Tungsten, W, 183.85

Heat measurements reported by the following were examined:

1. Nordmeyer and Bernoulli (-185° to 20°C) [52].
2. Dewar (20° to 80°K) [12].
3. Lange (26° to 91°K) [42].
4. Zwikker and Schmidt (92° to 2521°K) [71,72].
5. Bronson, Chisholm, and Dockerty (-20° to 501°C) [3].
6. Silvidi and Daunt (1.5° to 3.5°K) [61].
7. Horowitz and Daunt (2° to 20°K) [19].
8. Rayne (0.2° to 1°K) [56].
9. Waite, Craig, and Wallace (4° to 15°K) [68].
10. DeSorbo (13° to 93°K) [11].
11. Clusius and Franzosini (12° to 274°K) [7].
12. Grodspeed and Smith (20° to 100°C) [17].
13. Defacqz and Guichard (15° to 423°C) [10].
14. Corbino (800° to 1900°C) [9].
15. Pirani (340° to 1350°C) [55].
16. Worthing (1200° to 2400°K) [69,70].
17. Gaehr (1400° to 2500°K) [15].
18. Smith and Bigler (2368° to 2485°K) [63].
19. Bockstahler (2371° to 2486°K) [1].
20. Magnus and Danz (21° to 901°C) [44].
21. Magnus and Holzman (99° to 899°C) [45].
22. Jaeger and Rosenbohm (20° to 1604°C) [22,23,24].
23. Hoch and Johnston (0° to 2620°C) [18].

The low-temperature measurements of Horowitz and Daunt [19]; Waite, Craig, and Wallace [68]; and Clusius and Franzosini [7] were combined to obtain smoothed values of heat capacity between 0° and about 280°K. The heat measurements at higher temperatures of Bronson, Chisholm, and Dockerty [3]; Magnus and Holzman [45]; Jaeger and Rosenbohm [23,24]; and Hoch and Johnston [18] were fitted by means of the least squares method to a heat-capacity equation of the form: $C = A+BT+C/T+D/T^2$. The equation obtained is:

$$C = 5.9871 + 6.732 \times 10^{-4} T - 1.161 \times 10^2/T + 9.9 \times 10^2/T^2 .$$

The values of heat capacity from this equation and those from the low-temperature measurements were joined smoothly. The equation was extrapolated to obtain the thermal functions up to 3000°K. The value of S°_{298} obtained is 7.805 e.u. The value given by Kelley and King [33] is 7.80 ±0.10 e.u.

Tungsten Dioxide, WO_2, 215.8488

King, Weller, and Christensen [39] reported measurements of the low-temperature heat-capacity in the range 53° to 297°K and of the relative enthalpy from 298° to 1800°K. Values of heat capacity between 0° and 53°K were obtained from the Debye-Einstein heat-capacity function $C = D(^{330}/T) + E(^{527}/T) + E(^{889}/T)$ given by King et al. [39]. The enthalpy equation $H_T - H_{298.15} = 15.49T + 1.79 \times 10^{-3}T^2 + 2.80 \times 10^5T^{-1} - 5717$ given also by King et al. [39] was evaluated to obtain values of heat capacity above 300°K. The three sets of values of heat capacity were joined smoothly and the thermodynamic functions calculated from 0° to 2000°K. The value of S°_{298} obtained is 12.078 e.u. as compared with the value 12.08 ±0.07 e.u. given by King et al. [39]. The enthalpy change between 298.15° and 400°K, where some adjustments in the heat capacity were needed, was calculated to be 1465 cal/mole. The value tabulated by King et al. [39] is 1450 cal/mole. Their enthalpy equation gives 1466 cal/mole.

Tungsten Trioxide, WO_3, 231.8482

Russell [58] reported measurements of the mean heat capacity of tungsten trioxide in the range -189° to +47°C; and Seltz, Dunkerley, and DeWitt [59] reported measurements of the heat capacity from 63° to 299°K. Recently, King, Weller, and Christensen [39] reported measurements of the heat capacity in the range 53° to 296°K and of the enthalpy relative to 298°K up to 1836°K. The results of King et al. [39] were used to obtain the thermodynamic functions. Values of heat capacity between 0° and 53°K were obtained from the Debye-Einstein heat-capacity equation $C = D(^{223}/T) + 2E(^{463}/T) + E(^{1141}/T)$ given by King et al. [39], and the values from 300°K to 1050°K were obtained from the enthalpy equation:

$$H_T-H_{298.15} = 21.26T + 1.69 \times 10^{-3}T^2 + 4.42 \times 10^5T^{-1} - 7971 ,$$

given for the α-WO_3 by King et al. [39]. At 1050°K α-WO_3 is shown to transform into β-WO_3 with heat of transition of 410 cal/mole. The melting point of β-WO_3 given by King et al. [39] is 1745°K with the heat of fusion of 17,550 cal/mole. Thermodynamic functions were calculated up to 2000°K using the enthalpy equations:

$$H_T - H_{298.15} = 20.79T + 1.39 \times 10^{-3} T^2 - 6300 \quad ,$$

for β-WO_3 from 1050° to the melting point 1745°K and

$$H_T - H_{298.15} = 31.50T - 3240 \quad ,$$

for liquid WO_3 from 1745° to 2000°K, which are given by King et al. [39]. The value of S°_{298} obtained is 18.044 e.u. King et al. [39] calculated 18.15 ±0.12 e.u. which is also the value given by Kelley and King [33]. The slight discrepancy comes about from differences in the extrapolated values of heat capacity below 53°K. The enthalpy increment for the interval 298.15° to 400°K was calculated to be 1911 cal/mole. The enthalpy equation derived by King et al. [39] gives 1908 cal/mole. King et al. has tabulated, however, 1880 cal/mole, showing that the equation value is considerably higher than the experimental value in this range.

Magnesium Monotungstate, M_gWO_4, 272.1596

The low-temperature measurements in the range 53° to 296°K reported by King and Weller [38] were examined. No high-temperature measurements have been located. The Debye-Einstein heat-capacity equation:

$$C = D(233/T) + E(319/T) + 3E(587/T) + E(1270/T) \ ,$$

given by King and Weller [38] was used to obtain values of heat capacity between 0° and 53°K. Thermodynamic functions were calculated after joining the experimental data smoothly with the extrapolated values. The value of S°_{298} obtained is 24.184 e.u. as compared with the value 24.2 ±0.2 given by King and Weller [38].

Lithium Metatitanate, Li_2TiO_3, 109.7762

King [34] reported heat capacity measurements in the range 55° to 296°K. Christensen, Conway and Kelley [5] measured the relative enthalpy from 298° to 1856°K. The Debye-Einstein heat-capacity equation:

$$C = D(299/T) + 3E(495/T) + E(676/T) + E(1023/T) \ ,$$

given by King [34] was used to obtain values of heat capacity between 0° and 55°K. The enthalpy equation:

$$H_T - H_{298.15} = 33.16T + 2.06 \times 10^{-3} T^2 + 6.98 \times 10^5 T^{-1} - 12{,}411 \quad ,$$

given by Christensen et al. [5] was used to obtain values of heat capacity from 298° to 1485°K. These three sets of values of heat capacity were joined smoothly and the thermodynamic functions calculated.

Christensen et al. [5] reported a transition at 1485°K from α-Li_2TiO_3 to β-Li_2TiO_3 involving 2750 cal/mole. The melting point of β-Li_2TiO_3 was found to be 1820°K with the heat of fusion of 26,330 cal/mole. The enthalpy equations:

$$H_T - H_{298.15} = 30.20T + 4.00 \times 10^{-3}\, T^2 - 9070 \ ,$$

for β-Li_2TiO_3, and

$$H_T - H_{298.15} = 48.00T - 1890 \ ,$$

for liquid Li_2TiO_3 (1820° to 1856°K) were used to calculate the thermodynamic functions to 2000°K. The value of S^o_{298} obtained is 21.933 e.u. as compared with the value 21.9 ±0.1 e.u. given by King [34] and 21.93 ±0.10 e.u. given by Kelley and King [33]. The enthalpy increment obtained for the interval 298° to 400°K is 2927 cal/mole as compared with 2928 cal/mole from Christensen et al.'s enthalpy equation [5] and with 2900 cal/mole tabulated by Christensen et al.

Magnesium Metasilicate, $MgSiO_3$, 100.3962

Wagner [67] reported heat-capacity measurements on $MgSiO_3$ (clinoenstatite) for the range 21° to 35°K and enthalpy measurements for the range 14° to 1297°C. Kelley [31] reported also heat-capacity measurements on clinoenstatite from 53° to 295°K. The values of heat capacity from 0° to 53°K were obtained by evaluating the Debye-Einstein heat-capacity equation:

$$C = D(333/T) + 2E(494/T) + 2E(1058/T) \ ,$$

given by Kelley [31]. Above 300°K the enthalpy equation:

$$H_T - H_{298.15} = 24.55T + 2.37 \times 10^{-3}\, T^2 + 6.28 \times 10^5\, T^{-1} - 9637 \ ,$$

given by Kelley [32] in Bureau of Mines Bulletin 584 was used to obtain values of heat capacity. The thermodynamic functions from 0° to 2000°K were calculated using these three sets of values of heat capacity. The value of S^o_{298} obtained is 16.194 e.u. as compared with the value 16.2 ±0.2 e.u. given by Kelley [31] and 16.22 ±0.10 e.u. given by Kelley and King [33]. The enthalpy increment for the interval 298.15° to 400°K obtained is 2138 cal/mole. The enthalpy equation given by Kelley [32] yields 2132 cal/mole. The value tabulated by Kelley inthe Bureau of Mines Bulletin 584 [32] is 2140 cal/mole.

Magnesium Orthosilicate, Mg_2SiO_4, 140.7076

Kelley [31] measured the heat capacity of Mg_2SiO_4 (forsterite) from 53° to 295°K and Orr [53] the enthalpy from 298° to 1808°K. The values of heat capacity from 0° to 53°K were calculated from the Debye-Einstein heat-capacity function: C = D(310/T) + 4E(509/T), given by Kelley [31] and the values above 300°K were calculated from the enthalpy equation:

$$H_T-H_{298.15} = 35.81T + 3.27 \times 10^{-3} T^2 + 8.52 \times 10^5 T^{-1} - 13,825 ,$$

given by Orr [53]. The three sets of values of heat capacity were joined smoothly and the thermodynamic functions calculated from 0° to 2000°K. The value of S^o_{298} obtained is 22.737 e.u. as compared with the value 22.7 ±0.2 e.u. given by Kelley [31] and with the value 22.75 ±0.2 e.u. given by Kelley and King [33]. In the interval 298.15° to 400°K where a slight adjustment was made in the values of heat capacity derived from the enthalpy equation, the enthalpy increment was calculated to be 3153 cal/mole, whereas Orr's enthalpy equation [53] gives 3152 cal/mole. Orr [53] tabulated 3100 cal/mole for the interval.

Magnesium Metatitanate, $MgTiO_3$, 120.2102

Shomate [60] measured the heat capacity of $MgTiO_3$ from 53° to 296°K and Naylor and Cook [48] measured the relative enthalpy from 298° to 1720°K. Values of heat capacity from 0° to 53°K were obtained from the Debye-Einstein heat-capacity equation:
C = D(365/T) + E(383/T) + 3E(711/T), given by Shomate [60] and those above 300°K were obtained from the enthalpy equation:

$$H_T-H_{298.15} = 28.29T + 1.64 \times 10^{-3} T^2 + 6.530 \times 10^5 T^{-1} - 10,771 ,$$

given by Naylor and Cook [48]. The three sets of values of heat capacity were joined smoothly and the thermodynamic functions calculated from 0° to 2000°K. The value of S^o_{298} obtained is 17.825 e.u. as compared with 17.8 ±0.1 e.u. given by Shomate [60] and with 17.82 ±0.10 e.u. given by Kelley and King [33]. The enthalpy increment obtained for the interval 298.15° to 400°K is 2440 cal/mole. The enthalpy equation given by Naylor and Cook [48] also gives 2440 cal/mole. Naylor and Cook [48] tabulated 2500 cal/mole for the interval.

Magnesium Dititanate, $MgTi_2O_5$, 200.1090

Todd [66] measured the heat capacity of $MgTi_2O_5$ from 52° to 297°K and Orr and Coughlin [54] measured the relative enthalpy from 298° to 1812°K. Values of heat capacity between 0° and 52°K were obtained from the Debye-Einstein heat-capacity function:
C = D(246/T) + 4E(420/T) + 3E(906/T), given by Todd [66] and the values above 300°K from the enthalpy equation:

$$H_T-H_{298.15} = 40.68T + 4.60 \times 10^{-3} T^2 + 7.35 \times 10^5 T^{-1} - 15,000 ,$$

given by Orr and Coughlin [54]. The three sets of values of heat capacity were joined smoothly and the thermodynamic functions calculated from 0° to 2000°K. The value of S^{o}_{298} obtained is 30.416 e.u. Todd [66] and Kelley and King [33] give S_{298} = 30.4 ±0.2 e.u. The enthalpy increment obtained for the interval 298.15° to 400°K is 3843 cal/mole. The enthalpy equation derived by Orr and Coughlin [54] gives also 3843 cal/mole. The value tabulated by Orr and Coughlin [54] is 3780 cal/mole.

Magnesium Orthotitanate, Mg_2TiO_4, 160.5216

Todd [66] measured the heat capacity from 52° to 297°K and Orr and Coughlin [54] measured the relative enthalpy from 298° to 1819°K. Values of heat capacity from 0° to 52°K were obtained from the Debye-Einstein heat-capacity equation: C = D(305/T) + 3E(447/T) + 3E(823/T) given by Todd [66] and the values above 300°K were obtained from the enthalpy equation:

$$H_T - H_{298.15} = 35.96T + 4.27 \times 10^{-3}\ T^2 + 6.89 \times 10^{5}\ T^{-1} - 13{,}412\ ,$$

given by Orr and Coughlin [54]. Thermodynamic functions from 0° to 2000°K were calculated after joining smoothly the three sets of values of heat capacity. The value of S^{o}_{298} obtained is 26.134 e.u. which includes the residual entropy R ln 2 considered to be present in this variate-type spinel [37]. Kelley and King [33] give 26.1 ±0.2 e.u. The value 24.76 ±0.15 e.u. given by Todd [66] does not include the residual entropy. The enthalpy increment obtained for the interval 298.15° to 400°K is 3378 cal/mole. The value tabulated for the interval by Orr and Coughlin [54] is 3340 cal/mole and that calculated using their enthalpy equation is 3378 cal/mole.

Lead, Pb, 207.19

The following low-temperature heat- capacity data were examined:

1. Nernst (23° to 273°K) [49]
2. Eucken and Schwers (16° to 276°K) [14]
3. Griffiths and Griffiths (23° to 380°K) [16]
4. Keesom and Onnes (14° to 80°K) [28]
5. Keesom and Andrews (2° to 21°K) [25]
6. Keesom and Ende (2° to 20°K) [26,27]
7. Bronson and Wilson (-80° to 120°C) [4]
8. Meads, Forsythe, and Giauque (14° to 300°K) [46]
9. Clement and Quinnell (6° to 8°K) [6]
10. Horowitz, Silvidi, Malaker, and Daunt (1° to 75°K) [20].

Smoothed values of heat capacity were obtained from 0° to about 300°K from these data and combined with the high temperature relative enthalpy data reported by Douglas and Dever [13] from 0° to 895°C. Thermodynamic functions from 0° to 1200°K were calculated. The value of S°_{298} obtained is 15.477 e.u. as compared with the value 15.49 ±0.05 e.u. given by Kelley and King [33]. The enthalpy increment for the interval 298.15° to 400°K is 658 cal/mole. The tabulated value given by Douglas and Dever [13] is 656 cal/mole.

Lead Monoxide (Yellow), PbO, 223.1894

The following low-temperature heat-capacity measurements on yellow PbO have been reported:

1. Nernst and Schwers [50], 21° to 93°K.
2. King [35], 54° to 296°K.
3. Kostryukov and Morozova [41], 12° to 303°K.

Russell [58] reported measurements of the mean heat capacity over the complete range -191° to +44°C in three temperature increments. High-temperature relative enthalpy measurements were reported by the following:

1. Magnus [43], 16° to 271°C.
2. Spencer and Spicer [64], 25° to 650°C.
3. Rodigina, Gomel'skii, and Luginina [57], 293° to 1195°K.

The low-temperature data of Nernst and Schwers [50], King [35], and Kostryukov and Morozova [41] are in good agreement. The high-temperature data of Rodigina *et al.* [57] were found to be most compatible with these low-temperature data. Values of heat capacity between 0° and 12°K were obtained from the Debye-Einstein heat-capacity equation: $C = D(145/T) + E(473/T)$ given by King [35]. The values of heat capacity above 300°K were obtained from the enthalpy equation:

$$H_T - H_{293.15} = 11.078T + 1.356 \times 10^{-3} T + 0.853 \times 10^{5} T^{-1} - 3655 \quad ,$$

given by Rodigina *et al.* [57]. The melting point was taken to be 1170°K with the heat of fusion of 5983 cal/mole. The enthalpy equation:

$$H_T - H_{298.15} = 23.899T - 10{,}862 \quad ,$$

for the liquid, determined by fitting the experimental data by the method of least squares, was used to 2000°K. The value of S°_{298} obtained is 16.362 e.u. King [35] gives 16.1 ±0.2 e.u. for S°_{298}, Kostryukov and Morozova [41] 16.42 ±0.05 e.u., and Kelley and King [33] 16.1 ±0.2 e.u. The difference is caused primarily by the difference in S°_{51} which King [35] and Kelley and King [33] obtained completely by extrapolation, while the calculation of Kostryukov and Morozova [41] and of the work presented here involved extrapolation below 12°K only. The original enthalpy equations and experimental data given by Rodigina *et al.* [57] were in joules. The conversion to calories was made on the basis of 4.1840 j = 1 cal.

Lead Monoxide (Red), PbO, 223.1894

Heat-capacity measurements on red PbO have been reported by King [35] in the range 53° to 296°K. Spencer and Spicer [64] reported relative enthalpy measurements from 25° to 550°C with 400°C as the lowest temperature of measurement relative to 25°C. Analysis of the high-temperature data on the computer has yielded results considerably "out of line" with the low-temperature data, therefore the high-temperature data was not included in the calculation of the thermodynamic functions for the present report. Thermodynamic functions up to 300°K only were calculated. The values of heat capacity between 0° and 53°K were calculated from the Debye-Einstein heat-capacity function $C = (156/T) + E(481/T)$ given by King [35]. The calculated values of heat capacity and the experimental values were joined smoothly and the thermodynamic functions calculated from 0° to 300°K. The value of S°_{298} obtained is 15.584 e.u. as compared with the value 15.6 ±0.2 e.u. given by King [35] and by Kelley and King [33].

Lead Dioxide, PbO_2, 239.1888

Heat measurements on PbO_2 have been reported by Russell [58] (from -188° to 46°C) and by Millar [47] (from 70° to 297°K). The measurements of Russell [58] were made by the "method of mean heat capacity" covering the complete range in three temperature increments. The Debye-Einstein heat-capacity equation $C = D(183/T) + E(342/T)$ given by Millar [47] was used to obtain values of heat capacity between 0° and 70°K. These equation values were joined smoothly with Millar's experimental data and the thermodynamic functions calculated from 0° to 300°K. The value of S°_{298} obtained is 18.258 e.u. as compared with 18.27 given by Millar [47] and with 18.3 ±0.5 e.u. given by Kelley and King [33].

Lead Sesquioxide, Pb_2O_3, 462.3782

The only heat-capacity data found were those reported by King [35] in the range 53° to 297°K. The Debye-Einstein heat-capacity equation $C = D(79.4/T) + 2E(220/T) + 2E(653/T)$ given by King [35] was used to obtain values of heat capacity from 0° to 53°K. The experimental values of heat capacity were joined smoothly with the equation values and the thermodynamic functions were calculated between 0° and 300°K. The value of S°_{298} obtained is 36.232 e.u. as compared with the value 36.3 ±0.7 e.u. given by King [35] and by Kelley and King [33] in the Bureau of Mines Bulletin 592. The slight difference is caused by the smoothing adjustment of the extrapolated equation values of heat capacity below 51°K.

Lead Orthoplumbate, Pb_3O_4, 685.5676

The only experimental heat data found for Pb_3O_4 were those reported by Millar [47] for the range 72° to 293°K. The Debye-Einstein heat-capacity equation:
$C = D(145/T) + D(79.5/T) + E(473/T) + 2E(220/T) + 2E(653/T)$ was used to

obtain values of heat capacity between 0° and 72°K. The equation values were joined smoothly with the experimental values and the thermodynamic functions calculated from 0° to 300°K. The value of S°_{298} obtained is 51.720 e.u. as compared with the value 60.53 e.u. given by Millar [47] and 50.5 ±1.6 e.u. given by Kelley and King [33]. Kelley [29] in an earlier Bureau of Mines Bulletin 350 pointed out arithmetical error in Millar's evaluation of the entropy. The variation between the value given in this report and that given by Kelley and King [33] is caused by the extrapolated values of heat capacity below 72°K. This suggests that experimental measurements are needed below 72°K.

Lead Metasilicate, $PbSiO_3$, 283.2742

The measurements of King [36] in the range 53° to 296°K are the only heat data found for $PbSiO_3$. The Debye-Einstein heat-capacity equation $C = D(140/T) + E(213/T) + 2E(596/T) + E(1440/T)$ was used to obtain values of heat capacity between 0° and 53°K. The equation values were joined smoothly with the experimental values of King [36] and the thermodynamic functions calculated from 0° to 300°K. The value of S°_{298} obtained is 26.260 e.u. as compared with the value 26.2 ±0.3 e.u. given by King [36] and by Kelley and King [33].

Lead Orthosilicate, Pb_2SiO_4, 506.4636

The measurements by King [36] in the range 53° to 296°K are the only heat data found for Pb_2SiO_4. The values of heat capacity between 0° and 53°K were calculated from the Debye-Einstein heat-capacity equation $C = D(78.5/T) + 2E(164/T) + 3E(547/T) + E(1379/T)$ given by King [36] and joined smoothly with his experimental values. Thermodynamic functions were calculated from 0° to 300°K. The value of S°_{298} obtained is 44.529 e.u. as compared with the value 44.6 ±0.5 e.u. given by King [36] and by Kelley and King [33].

Aluminum Silicate, Al_2SiO_5, 162.0460

Aluminum silicate, Al_2SiO_5, exists in nature in three known crystalline forms identified as andalusite, kyanite, and sillimanite. Simon and Zeidler [62] and Todd [65] have reported heat-capacity measurements on all three of these substances. The ranges of their measurements are as follows:

	Simon and Zeidler	Todd
Andalusite	24° to 280°K	54° to 297°K
Kyanite	24° to 224°K	54° to 297°K
Sillimanite	17° to 282°K	54° to 297°K.

High-temperature relative enthalpy measurements have been reported by the following:

Andalusite:

Neumann [51], from 0° to 1300°C.

Kyanite:

a. Neumann [51], 0° to 1400°C.

b. Kolossowsky and Skoulski [40], 16° to 342°C.

Sillimanite:

a. Neumann [51], 0° to 1300°C.

b. Cohn [8], 20° to 1400°C.

The high-temperature relative enthalpy data were found to be considerably "out of line" with the low-temperature data and were thus not included in the calculation of the thermodynamic functions for this report. The thermodynamic functions for these substances are given only up to 300°K. The data reported by Simon and Zeidler [62] differed almost 100 percent at the lower temperatures from those reported by Todd [65]. The data given by Todd [65] were accepted. Values of heat capacity from 0° to about 55°K were obtained by evaluating the following Debye-Einstein heat-capacity equations given by Todd [65]:

Andalusite:

$$C = D(311/T) + 3E(485/T) + 4E(1035/T)$$

Kyanite:

$$C = D(395/T) + 3E(569/T) + 4E(1271/T)$$

Sillimanite:

$$C = D(292/T) + 3E(468/T) + 4E(1048/T) .$$

The equation and the experimental values of heat capacity were smoothed and the thermodynamic functions calculated. The values of S°_{298} obtained are compared with those given by Todd [65] and by Kelley and King [33]:

	This Work cal/deg mole	Todd cal/deg mole	Kelley and King cal/deg mole
Andalusite	22.279	22.28 ±0.10	22.28 ±0.10
Kyanite	20.027	20.02 ±0.08	20.02 ±0.08
Sillimanite	22.988	22.97 ±0.10	22.97 ±0.10 .

Beryllium Orthosilicate, Be_2SiO_4, 110.1080

The only heat data found on Be_2SiO_4 were those reported by Kelley [30] between 55° and 294°K. The Debye-Einstein heat-capacity function $C = D(422/T) + 2E(527/T) + 4E(1135/T)$ given by Kelley [30] was used to obtain values of heat capacity between 0° and 55°K. Thermodynamic functions were calculated between 0° and 300°K after smoothly joining the equation and experimental values of heat capacity. The value of S^o_{298} obtained is 15.338 e.u. as compared with 15.4 ±0.1 e.u. given by Kelley [30] and with 15.37 ±0.08 e.u. given by Kelley and King [33].

Aluminum Titanate, Al_2TiO_5, 181.86

King [34] reported heat-capacity measurements in the range 53° to 296°K on the β form of Al_2TiO_5. Bonnickson [2] determined the relative enthalpy from 298° to 1803°K. The Debye-Einstein heat-capacity function $C = D(276/T) + 4E(477/T) + 3E(1049/T)$ given by King [34] was used to obtain values of heat capacity between 0° and 53°K. The values of heat capacity above 300°K were obtained from the enthalpy equation:

$$H_T - H_{298.16} = 43.63T + 2.65 \times 10^{-3}T^2 + 11.21 \times 10^5T^{-1} - 17{,}004\ ,$$

given by Bonnickson [2]. The three sets of values of heat capacity were joined smoothly and the thermodynamic functions from 0° to 2000°K calculated. The value of S^o_{298} obtained is 26.165 e.u. as compared with the value 26.2 ±0.2 e.u. given by King [34] and by Kelley and King [33]. The enthalpy change for the interval 298.15° to 400°K was calculated to be 3674 cal/mole. The enthalpy equation given by Bonnickson [2] yields 3675 cal/mole. Bonnickson's tabular value [2], which is considered closely representative of the experimental data, is 3600 cal/mole.

COMPARISON OF VALUES OF S°_{298}
(In cal/deg mole)

Substance	This Work	Original Paper	Kelley and King [33]
W	7.805	8.2 ±0.2 [11] 7.83 [7]	7.80 ±0.10
WO_2	12.078	12.08 ±0.07 [39]	12.08 ±0.07
WO_3	18.044	19.90 ±0.2 [59] 18.15 ±0.12 [39]	18.15 ±0.12
$MgWO_4$	24.184	24.2 ±0.2 [38]	- -
Li_2TiO_3	21.933	21.9 ±0.1 [34]	21.93 ±0.10
$MgSiO_3$ (clinoenstatite)	16.194	16.2 ±0.2 [31]	16.22 ±0.10
Mg_2SiO_4	22.737	22.7 ±0.2 [31]	22.75 ±0.2
$MgTiO_3$	17.825	17.8 ±0.1 [60]	17.82 ±0.10
$MgTi_2O_5$	30.416	30.4 ±0.2 [66]	30.4 ±0.2
Mg_2TiO_4	26.134	24.76 ±0.15 [66]	26.1 ±0.2
Pb	15.477	15.514 [46]	15.49 ±0.05
PbO (yellow)	16.362	16.1 ±0.2 [35] 16.42 ±0.05 [41]	16.1 ±0.2
PbO (red)	15.584	15.6 ±0.2 [35]	15.6 ±0.2
PbO_2	18.258	18.27 [47]	18.3 ±0.5
Pb_2O_3	36.232	36.3 ±0.7 [35]	36.3 ±0.7
Pb_3O_4	51.720	60.53 [47]	50.5 ±1.6
$PbSiO_3$	26.260	26.2 ±0.3 [36]	26.2 ±0.3
Pb_2SiO_4	44.529	44.6 ±0.5 [36]	44.6 ±0.5
Al_2SiO_5			
Andalusite	22.279	22.28 ±0.10 [65]	22.28 ±0.10
Kyanite	20.027	20.02 ±0.08 [65]	20.02 ±0.08
Sillimanite	22.988	22.97 ±0.10 [65]	22.97 ±0.10
Be_2SiO_4	15.338	15.4 ±0.1 [30]	15.37 ±0.08
Al_2TiO_5	26.165	26.2 ±0.2 [34]	26.2 ±0.2

References

1. L. I. Bockstahler, The Specific Heat of Incandescent Tungsten by an Improved Method, Phys. Rev. 25, 677-685 (1925).

2. K. R. Bonnickson, High Temperature Heat Contents of Some Titanates of Aluminum, Iron, and Zinc, J. Am. Chem. Soc. 77, 2152-2154 (1955).

3. H. L. Bronson, H. M. Chisholm, and S. M. Dockerty, On the Specific Heats of Tungsten, Molybdenum, and Copper, Can. J. Research 8, 282-303 (1933).

4. H. L. Bronson and A. J. C. Wilson, The Heat Capacities of Silver, Nickel, Zinc, Cadmium, and Lead from -80° to 120°C, Can. J. Research 14A, 181-193 (1936)..

5. A. U. Christensen, K. C. Conway, and K. K. Kelley, High-Temperature Heat Contents and Entropies of Aluminates and Ferrites of Lithium and Sodium, and of Lithium Titanate, Bureau of Mines Report of Investigations No. 5565, 1960.

6. J. R. Clement and E. H. Quinnell, The Atomic Heat of Lead in the Region of the Transition to Superconductivity, Phys. Rev. 85, 502-503 (1952).

7. K. Clusius and P. Franzosini, Ergebnisse der Tieftemperaturforschung. XXIII. Atom - und Elektronenwärme des Molybdäns und Wolframs zwischen 10°K und 273°K, Z. Naturforsch. 14A, 99-105 (1959).

8. W. Cohn, The Problem of Heat Economy in the Ceramic Industry. II, J. Am. Ceramic Soc. 7, 475-488 (1924).

9. O. M. Corbino, Über die spezifische Wärme der Metalle bei hohen Temperaturen, Physik. Zeit. 13, 375-383 (1912).

10. E. Defacqz and M. Guichard, Sur la Détermination de la Chaleur Spécifique du Tungstène et du Molybène, Ann. Chim. Phys. [7] 24, 139-144 (1901).

11. W. DeSorbo, Low Temperature Heat Capacity of Bismuth and Tungsten, J. Phys. Chem. 62, 965-967 (1958).

12. J. Dewar, Atomic Specific Heats between the Boiling Points of Liquid Nitrogen and Hydrogen. I. The Mean Atomic Specific Heats at 50° Absolute of the Elements a Periodic Function of the Atomic Weights, Proc. Roy. Soc. (London) 89A, 158-169 (1913).

13. T. B. Douglas and J. L. Dever, Heat Content of Lead from 0° to 900°, and the Heat of Fusion, J. Am. Chem. Soc. 76, 4824-4826 (1954).

14. A. Eucken and F. Schwers, Eine experimentelle Prüfung des T^3-Gesetzes für den Verlauf der spezifischen Wärme fester Körper bei tiefen Temperaturen, Ber. deut. physik. Ges. 15, 578-588 (1913).

15. P. F. Gaehr, The Specific Heat of Tungsten at Incandescent Temperatures, Phys. Rev. 12, 396-423 (1918).

16. E. H. Griffiths and E. Griffiths, The Capacity for Heat of Metals at Low Temperatures, Proc. Roy. Soc. (London) 90A, 557-560 (1914).

17. A. W. Grodspeed and E. F. Smith, Über die spezifische Wärme des metallischen Wolframs, Zeit. anorg. Chem. 8, 207-212 (1895).

18. M. Hoch and H. L. Johnston, A High Temperature Drop Calorimeter. The Heat Capacities of Tantalum and Tungsten between 1000° and 3000°K, J. Phys. Chem. 65, 855-860 (1961).

19. M. Horowitz and J. G. Daunt, The Electronic and Lattice Specific Heats in W, Mo, and Re, Phys. Rev. 91, 1099-1106 (1953).

20. M. Horowitz, A. A. Silvidi, S. F. Malaker, and J. G. Daunt, The Specific Heat of Lead in the Temperature Range 1°K to 75°K, Phys. Rev. 88, 1182-1186 (1952).

21. "IUPAC Revises Atomic Weight Values", Chem. Eng. News 39, 42-43 (1961).

22. F. M. Jaeger and E. Rosenbohm, La Détermination Exacte des Chaleurs Spécifiques des Corps Solides aux Températures entre 0° et 1625°C, Rec. trav. chim. 47, 513-557 (1928).

23. F. M. Jaeger and E. Rosenbohm, The Exact Measurement of the Specific Heats of Solid Substances at High Temperatures. III. The Specific Heats of Palladium and of Tungsten, Proc. Acad. Sci. Amsterdam 33, 457-472 (1930).

24. F. M. Jaeger and E. Rosenbohm, La Détermination Exacte des Chaleurs Spécifiques Vrais du Tungstène, du Rhodium, du Palladium, du Ruthénium, de l'Osmium et de l'Iridium à des Températures entre 0° et 1625°C, Rec. trav. chim. 51, 1-46 (1932).

25. W. H. Keesom and D. H. Andrews, The Specific Heats of Solid Substances at the Temperatures Attainable with the Help of Liquid Helium. I. Measurements of the Atomic Heat of Lead, Comm. Phys. Lab. Univ. Leiden, No. 185a, 2-13 (1927).

26. W. H. Keesom and J. N. van den Ende, The Specific Heat of Solid Substances at the Temperatures Obtainable with the Aid of Liquid Helium. II. Measurements of the Atomic Heats of Lead and Bismuth, Proc. Acad. Sci. Amsterdam 33, 243-245 (1930); Comm. Phys. Lab. Univ. Leiden No. 203d, 25-38 (1930).

27. W. H. Keesom and J. N. van den Ende, The Specific Heat of Solid Substances at the Temperatures Obtainable with the Aid of Liquid Helium. III. Measurements of the Atomic Heats of Lead and Bismuth. A Correction, Proc. Acad. Sci. Amsterdam 34, 210-211 (1931); Comm. Phys. Lab. Univ. Leiden No. 213c, 27-31 (1931).

28. W. H. Keesom and H. K. Onnes, The Specific Heat at Low Temperatures. I. Measurements on the Specific Heat of Lead between 14° and 80°K and of Copper between 15° and 22°K, Comm. Phys. Lab. Univ. Leiden No. 143, 13, 2-26 (1914).

29. K. K. Kelley, Contributions to the Data on Theoretical Metallurgy. I. The Entropies of Inorganic Substances, U. S. Bureau of Mines Bulletin 350 (1932).

30. K. K. Kelley, The Specific Heats at Low Temperatures of Beryllium Oxide and Beryllium Orthosilicate (Phenacite), J. Am. Chem. Soc. 61, 1217-1218 (1939).

31. K. K. Kelley, Specific Heats at Low Temperatures of Magnesium Orthosilicate and Magnesium Metasilicate, J. Am. Chem. Soc. 65, 339-341 (1943).

32. K. K. Kelley, Contributions to the Data on Theoretical Metallurgy. XIII. High-Temperature Heat-Content, Heat-Capacity, and Entropy Data for the Elements and Inorganic Compounds, Bureau of Mines Bulletin 584, 1960.

33. K. K. Kelley and E. G. King, Contributions to the Data on Theoretical Metallurgy. XIV. Entropies of the Elements and Inorganic Compounds, U. S. Bureau of Mines Bulletin No. 592, 1961.

34. E. G. King, Low-Temperature Heat Capacities and Entropies at 298.16°K of Some Titanates of Aluminum, Calcium, Lithium and Zinc, J. Am. Chem. Soc. 77, 2150-2152 (1955).

35. E. G. King, Low-Temperature Heat Capacities and Entropies at 298.15°K of Lead Sesquioxide and Red and Yellow Lead Monoxide, J. Am. Chem. Soc. 80, 2400-2401 (1958).

36. E. G. King, Low-Temperature Heat Capacities and Entropies at 298.15°K of Crystalline Lead Metasilicate, Lead Orthosilicate and Cadmium Metasilicate, J. Am. Chem. Soc. 81, 799-800 (1959).

37. E. G. King and K. K. Kelley, Low-Temperature Heat Capacities of Copper Ferrites (with a Summary of Entropies at 298.15°K of Spinel Minerals), Bureau of Mines Report of Investigations No. 5502, 1959.

38. E. G. King and W. W. Weller, Low-Temperature Heat Capacities and Entropies at 298.15°K of Monotungstates of Sodium Magnesium and Calcium, U. S. Bureau of Mines Report of Investigations No. 5791, 1961.

39. E. G. King, W. W. Weller, and A. U. Christensen, Thermodynamics of Some Oxides of Molybdenum and Tungsten, U. S. Bureau of Mines Report of Investigations No. 5664, 1960.

40. N. A. Kolossowsky and Ida Skoulski, Sur les écarts de la loi de Neumann, Joule et Kopp et sur la chaleur moléculaire apparente de l'eau dans les combinaisons solides, Bull. Soc. Chim. (France) (4) 47, 136-147 (1930).

41. V. N. Kostryukov and G. Kh. Morozova, Thermodynamic Studies at Low Temperatures. X. Heat Capacity of the Yellow Modification of Lead Oxide between 12.5° and 303°K and Its Entropy at 298.15°K, Zhurnal Fiz. Khim. 34, 1833-1836 (1960); Russian J. Phys. Chem. 34, 873-874 (1960).

42. F. Lange, Untersuchungen über die spezifische Wärme bei tiefen Temperaturen, Z. physik. Chem. 110, 343 (1924).

43. A. Magnus, Messungen spezifischer Wärmen fester Körper bei hohen Temperaturen, Physik. Zeit. 14, 5-11 (1913).

44. A. Magnus and H. Danz, Die spezifische Wärme von Wolfram, Bor, Borstickstoff und Berylliumoxyd, Ann. Physik (4) 81, 407-424 (1926).

45. A. Magnus and H. Holzmann, Untersuchungen über die spezischen Wärmen von Tantal, Wolfram, und Beryllium zwischen 100 und 900°C, Ann. Physik (5) 3, 585-613 (1929).

46. P. F. Meads, W. R. Forsythe, and W. F. Giauque, The Heat Capacities and Entropies of Silver and Lead from 15° to 300°K, J. Am. Chem. Soc. 63, 1902-1905 (1941).

47. R. W. Millar, The Heat Capacities at Low Temperatures of the Oxides of Tin and Lead, J. Am. Chem. Soc. 51, 207-214 (1929).

48. B. F. Naylor and O. A. Cook, High Temperature Heat Contents of the Metatitanates of Calcium, Iron and Magnesium, J. Am. Chem. Soc. 68, 1003-1005 (1946).

49. W. Nernst, Der Energieinhalt fester Stoffe, Ann. Physik (4) 36, 395-439 (1911).

50. W. Nernst and F. Schwers, Untersuchungen über die spezifische Wärme bei tiefen Temperaturen. VIII, Sitzber. könig. preuss. Akad. Wiss. 1914, 355-370 (1914).

51. F. Neumann, Über die Stabilitätsverhältnisse der Modifikationen im polymorphen System $A\ell_2SiO_5$, Zeit. anorg. Chem. 145, 193-238 (1925).

52. P. Nordmeyer and A. L. Bernoulli, Determination of the Specific Heat of Some Elements, Alloys, and Compounds between -185° and 20°C, Verhandl. deut. physik. Ges. 9, 175-183 (1907).

53. R. L. Orr, High Temperature Heat Contents of Magnesium Orthosilicate and Ferrous Orthosilicate, J. Am. Chem. Soc. 75, 528-529 (1953).

54. R. L. Orr and J. P. Coughlin, High Temperature Heat Contents of Magnesium Orthotitanate and Magnesium Dititanate, J. Am. Chem. Soc. 74, 3186-3187 (1952).

55. M. v. Pirani, Über die Messung der spezifischen Wärme fester Körper bei hohen Temperaturen, Ber. deut. physik. Ges. 10, 1037-1054 (1912).

56. J. Rayne, Specific Heat of Metals Below One Degree Absolute, Phys. Rev. 95, 1428-1434 (1954).

57. E. N. Rodigina, K. Z. Gomel'skii, and V. F. Liginina, Entropy and Heat Capacity of Yellow Lead Oxide at High Temperatures, Zhurnal Fiz. Khim. 35, 1799-1802 (1961); Russian J. Phys. Chem. 35, 884-886 (1961).

58. A. S. Russell, Messungen von spezifischen Wärmen bei tiefen Temperaturen, Physik. Zeit. 13, 59-64 (1912).

59. H. Seltz, F. J. Dunkerley, and B. J. DeWitt, Heat Capacities and Entropies of Molybdenum and Tungsten Trioxides, J. Am. Chem. Soc. 65, 600-602 (1943).

60. C. H. Shomate, Heat Capacities at Low Temperatures of the Metatitanates of Iron, Calcium and Magnesium, J. Am. Chem. Soc. 68, 964-966 (1946).

61. A. A. Silvidi and J. G. Daunt, Electronic Specific Heats in Tungsten and Zinc, Phys. Rev. 77, 125-129 (1950).

62. F. Simon and W. Zeidler, Untersuchungen über der spezifischen Wärmen bei tiefen Temperaturen. (a) Die spezifischen Wärmen von Natrium, Kalium, Molybdän und Platin. (b) Bemerkung über die Abweichung der chemischen Konstanten einatomiger Gase vom theoretischen Wert, Zeit. physik. Chem. 123, 383-405 (1926).

63. K. K. Smith and P. W. Bigler, Oscillations of Temperature of an Incandescent Filament, and the Specific Heat of Tungsten, Phys. Rev. 19, 268-270 (1922).

64. H. M. Spencer and W. M. Spicer, The Heat Capacities of Red and Yellow Lead Monoxides at High Temperatures, J. Am. Chem. Soc. 64, 617-621 (1942).

65. S. S. Todd, Heat Capacities at Low Temperatures and Entropies at 298.16°K of Andalusite, Kyanite, and Sillimanite, J. Am. Chem. Soc. 72, 4742-4743 (1950).

66. S. S. Todd, Low Temperature Heat Capacities and Entropies at 298.16°K of Magnesium Orthotitanate and Magnesium Dititanate, J. Am. Chem. Soc. 74, 4669-4670 (1952).

67. H. Wagner, Zur Thermochemie der Metasilikate des Calciums und Magnesiums und des Diopsids, Zeit. anorg. allgem. Chem. 208, 1-22 (1932).

68. T. R. Waite, R. S. Craig, and W. E. Wallace, Heat Capacity of Tungsten between 4 and 15°K, Phys. Rev. 104, 1240-1241 (1956).

69. A. G. Worthing, Atomic Heats of Tungsten and of Carbon at Incandescent Temperatures, Phys. Rev. 12, 199-225 (1918).

70. A. G. Worthing, Atomic Heats of Tungsten and of Carbon at Incandescent Temperatures, J. Franklin Inst. 185, 707-708 (1918).

71. C. Zwikker, Messungen der spezifischen Wärme von Wolfram zwischen 90 und 2600° abs., Z. Physik 52, 668-77 (1928).

72. C. Zwikker and G. Schmidt, Metingen over de Soortelijke Warmte van Wolfraam tusschen 90 en 2600° Absoluut, Physica 8, 329-346 (1928).

Chapter B-8

THE DISSOCIATION ENERGY OF BeF

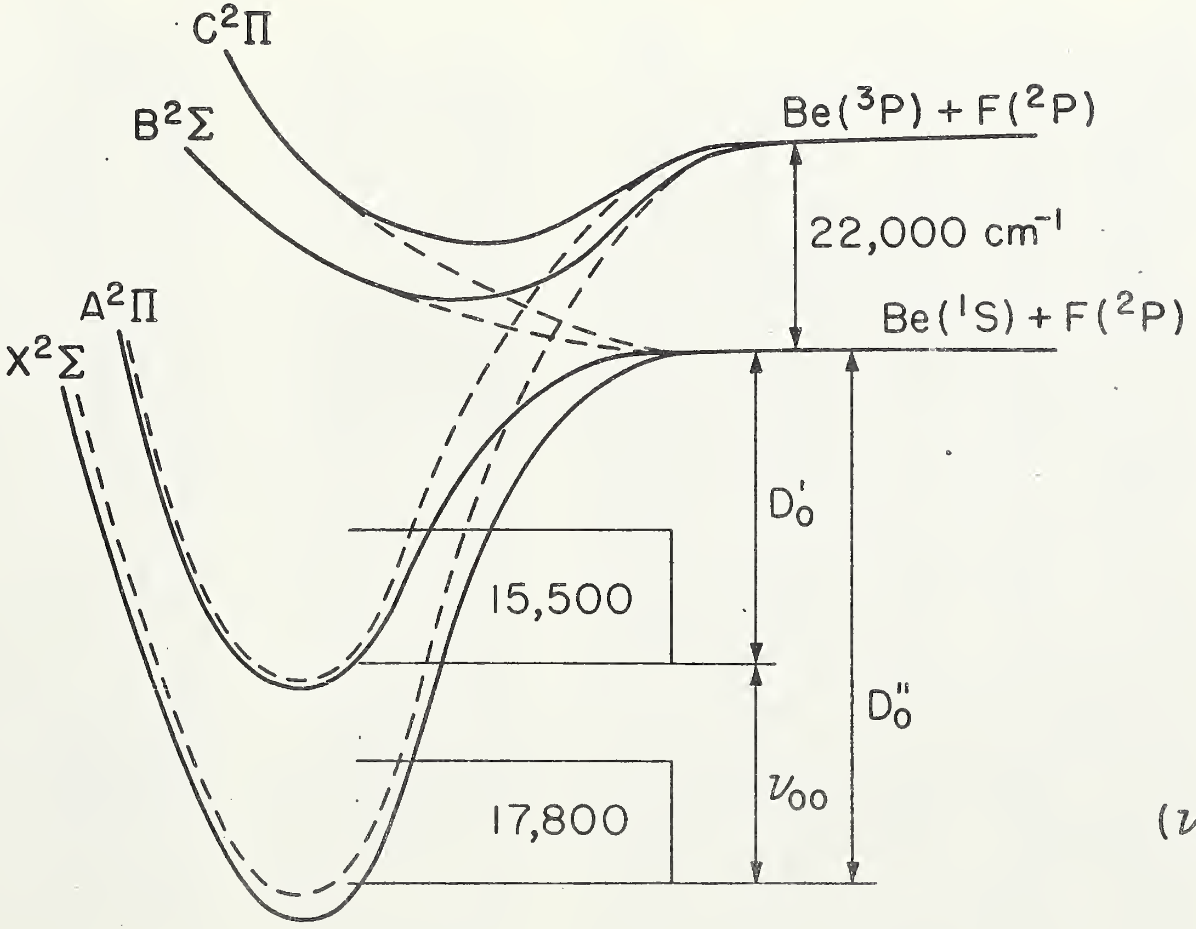
by D. E. Mann

Molecular Spectroscopy Section

In common with a good many other diatomic molecules whose electronic spectra have been investigated to only a limited extent the dissociation energy of the beryllium fluoride molecule, BeF, is quite uncertain. On the basis of early data, principally Jevons' analysis[1] of the Q_1 heads of some 20 bands of the $A^2\Pi-X^2\Sigma^+$ system observed in emission with relatively low resolution by Datta[2], and Jenkins' high resolution study of a few bands[3], the values 5.4 and 4±1 e.v. have been indicated for the dissociation energy of BeF in the X state. The former, listed by Herzberg[4] and Rosen[5], is simply the value obtained by a linear Berge-Sponer extrapolation ($D_0 = \omega_0^2/4x_0\omega_0$) of Jevons' data; the latter, given by Gaydon, is also based on this approximation but presumably takes into account his estimate of the probable net effect of ionic binding forces and the fact that the normal state of Be is $^1S_0$. More recently the obvious heads of a much larger number of bands of the A-X system of BeF have been measured in emission by Tatevskii, et al.[7]. They were led on the basis of their analysis of the vibrational structure to propose the much higher value 8.0 ±0.5 e.v. In view of the current interest in the properties of BeF it is worthwhile to reconsider briefly the various discrepant values which have been proposed and the evidence on which they are based.

The source of the middle value, 5.4 e.v., has already been noted. The use of the newer values[7] for ω_0 and $x_0\omega_0$ in place of those derived by Jevons would not change D_0 significantly. Gaydon has pointed out that in molecules in which ionic binding is important the linear Berge-Sponer extrapolation usually give results which are much too low, and that in molecules which dissociate to normal products one of which has a $^1S_0$ ground state the results often tend to be too high. His estimate of the balance between these two opposing effects led him to lower the linear result to 4 ±1 e.v.

In the Russian work the vibrational constants were determined by least-squares fitting the Q_1 heads in some 63 bands, with quantum numbers ranging up to 16 for the lower state and 15 for the upper, to a formula which includes terms in $y_0\omega_0$. The maximum discrepancy between observed and calculated head positions is about 3 cm^{-1}. Linear extrapolation gives 39,600 cm^{-1} and 42,900 cm^{-1} for D_0 in the A and X states respectively. Inclusion of the effect of the $y_0\omega_0$ term gives, according to Tatevskii, et al., 38,200 and 57,500 cm^{-1} respectively. Application of the non-crossing rule leads Tatevskii, et al. to propose the potential curve diagram shown here in Fig. 1, where the dashed lines give the "first-approximation" curves, and the solid lines the curves obtained after interaction is taken



$(\nu_{00} \simeq 33,000\ cm^{-1})$

Fig. 1 Potential Curves for BeF, after TATEVSKII, et al.

into account. It should be noticed that the A and X states are both supposed to dissociate to the same limit. In this circumstance the expression[8] relating (approximately) the energy separation, ν_{oo}, of the two states, their dissociation energies, D_o' and D_o'', and the energy difference of the atomic products, E_{atom}, viz., $\nu_{oo} + D' = D'' + E_{atom}$, becomes simply $\nu_{oo} = D'' - D'$. The difference of the extrapolated results, 57,500 - 38,200 = 19,300, does not agree with $\nu_{oo} = 33,000$. Tatevskii, et al. therefore arbitrarily increased D_o'' to 64,000 cm^{-1} and lowered D_o' to 31,000 cm^{-1} in order to obtain the difference ν_{oo}. This, in substance, is the source and derivation of their reported values for the dissociation energy of BeF in the A and X states, viz. 3.9 ±0.5 and 8.0 ±0.5 e.v., respectively.

The results given above are open to serious question on several counts.

A. The total vibrational energy G(v) at the highest levels observed is about 15,500 cm^{-1} for the A state and 18,800 cm^{-1} for the X state. For the latter this represents only about 30% of their adjusted, extrapolated value. The length of extrapolation alone would cast doubt on the reliability of their final value.

B. Adherence to the non-crossing rule frequently causes considerable distortion of the interacting curves, especially in the region of the higher levels, so that the justification for a simple extrapolation is again open to serious question. This is clear from the poor agreement between their difference $D_o'' - D_o'$ and ν_{oo}.

C. Despite the fact that the spectrum consists of marked sequences, that both the vibrational frequencies (and force constants) and internuclear distances are known to be very similar for the A and X states[3], Tatevskii, et al. propose on the basis of their analysis an enormous difference in dissociation energies. This is at best rather unlikely. Their result implies, moreover, that the higher-order curvature factors for the A state must be very important, thereby removing the justification for their simple extrapolation on the basis of their own conclusions.

D. The large difference between dissociation energies for the A and X states, which incidentally leads to that for the ground state being abnormally large, results largely from an implicit assumption they have made without either recognizing its consequences or justifying its use. They have assumed that the $A^2\Pi$ and $X^2\Sigma^+$ states both dissociate to the same products. This is a crucial point for if it is not true then their conclusions regarding the dissociation limits become erroneous.

It is certain that the observed transition is $^2\Pi_i - {}^2\Sigma^+$, and from Fowler's work[9] it is known that $^2\Sigma^+$ is in fact the ground state. Moreover, it is almost certainly true that the $^2\Sigma^+$ state dissociates to normal products, Be(^1S_o) and F(^2P). It is by no means certain, however, that the $^2\Pi_i$ state involved in the observed transition also dissociates to normal products. It may equally well be correlated with Be(^3P) + F(^2P), which lies about 22,000 cm^{-1} above the normal products. In this circumstance the relation $\nu_{00} + D' = D'' + E_{atom}$ would give 11,000 cm^{-1} as the difference between dissociation energies of the two states. There is evidence from the spectra of other second-group molecules and from the spectra of molecules isoelectronic with BeF that the present suggestion is correct. This will be discussed more fully elsewhere. If the two extrapolation limits for the A state are averaged one obtains about 38,900 cm^{-1}, while the average for X is 50,200 cm^{-1}. Their difference, 11,300 cm^{-1}, is in good agreement with the difference $\nu_{00} - E_{atom}$ = 11,000 cm^{-1}. On this basis $D_0'' \simeq$ 6.2 e.v. or 143 kcal/mole and $D_0' \simeq$ 4.8 e.v. or 111 kcal/mole. The heat of atomization of BeF_2(g) is approximately 300 kcal, or approximately 150 kcal per bond.

Another means of estimating the range within which D_0'' may lie is afforded by Fowler's observation that BeF_2 vapor did not produce detectable BeF spectra of the A-X system until about 1500°C. If the reasonable assumption is made that the lower limit for detection of BeF under Fowler's experimental conditions is 10^{-6} atm., the available thermochemical quantities for BeF_2, Be, and F_2 at 1750°K lead to D_0'' (BeF) $\simeq$ 140 kcal/mole. (See Chapter B-9.) A lower limit for detection of 10^{-7} atm. at 1750°K leads to about 124 kcal/mole, while 10^{-5} atm. leads to about 156 kcal/mole. Since Fowler also studied MgF_2 (among other Group II fluorides) and found MgF at 1350°C, the internal consistency is reasonable.

Although estimates of the dissociation energy of BeF could be arrived at in other ways it is the author's view that foregoing analysis serves to indicate, first, the unreliability of the new Russian result and, second, to suggest that D_0'' (BeF) is probably not far from 6 e.v., and possibly within the limits ±10%. A similar analysis has been made for other Group II halides and will be presented elsewhere.

References

1. W. Jevons, Proc. Roy. Soc. (London) A122, 216 (1929).

2. S. Datta, Proc. Roy. Soc. (London) A101, 187 (1922).

3. F. A. Jenkins, Phys. Rev. 35, 315 (1930).

4. G. Herzberg, Spectra of Diatomic Molecules (D. Van Nostrand Company, Inc., New York, 2nd Edition, 1950), Table 39.

5. B. Rosen, Editor, Tables de Constantes Sélectionies 4. Données spectroscopiques concernant les molécules diatomiques (Hermann et Cie, Paris, 1951).

6. A. G. Gaydon, Dissociation Energies (Chapman and Hall, Ltd., London, 2nd Edition, revised, 1953), p. 221.

7. V. M. Tatevskii, L. N. Tunitskii, and M. M. Novikov, Optika i Spektroskopiia, 5, No. 5, 520 (1958).

8. W. Jevons, Band Spectra of Diatomic Molecules (The Physical Society, London, 1932), p. 197.

9. C. A. Fowler, Jr., Phys. Rev. 59, 645 (1941).

Chapter B-9

GRAPHS SHOWING THE STABILITY OF GASEOUS BeF, $A\ell F$, $A\ell C\ell$, AND $A\ell C\ell_2$ AT VARIOUS TEMPERATURES AND PRESSURES

by Thomas B. Douglas, John E. Neufer, and W. Gary Goodson

Thermodynamic data and direct observation show that the subfluorides and subchlorides of beryllium and aluminum are in general sufficiently abundant to be important gaseous species in many high-temperature systems containing the pertinent chemical elements. Under given conditions the equilibrium partial pressure of such a gas is related thermodynamically in a straightforward way to its standard heat of formation (or dissociation energy), its ideal-gas free-energy function, and its gas imperfection. Though these gases are invariably assumed for simplicity (and usually with good approximation) to be ideal, and their computed free-energy functions are in most cases based on partly or wholly estimated molecular constants, the standard heat of formation is often by far the most uncertain piece of basic data in determining the equilibrium pressure of the gas.

Certain phases of the Bureau's light-element experimental program are currently concerned with these subhalide species in this connection in one of two ways, either (a) to choose conditions which will lead to appropriate pressures of them to permit measurement of their properties (spectroscopic, etc.), or (b) to investigate their equilibrium pressures as one of the best means of determining (or setting limits to) their standard heats of formation. Because of these interests (at NBS and elsewhere), we have for BeF, $A\ell F$, $A\ell C\ell$, and $A\ell C\ell_2$ taken the simplest system from which the subhalide can conveniently arise (the saturated halide plus the free metal) and have constructed graphs of the subhalide equilibrium pressures over a range of temperatures (and also total pressures in the case of the aluminum chlorides), using basic data for them as recorded in previous reports on this program and the more recent literature.

No graph was prepared for the important gas $BeC\ell$ pending subsequent preparation of a table of thermodynamic functions of the condensed phases of $BeC\ell_2$. Such a table for $BeC\ell_2$ has been prepared at the Bureau by correlation of molecular-constant, vapor-pressure, and vapor-density data, but final adjustments await the availability of condensed-state enthalpy data on the condensed phases currently being obtained by the Thermal Laboratory of the Dow Chemical Company.

The equilibrium pressures computed are shown in Fig. 1 for BeF, in Fig. 2 for AℓF, in Figs. 3a and 3b for AℓCℓ, and in Figs. 4a and 4b for AℓCℓ_2. In the cases of BeF and AℓF, the generating systems chosen were the condensed phases BeF_2 + Be and $A\ell F_3$ + Aℓ respectively (solid or liquid, depending on the temperature). The two condensed phases were assumed to be immiscible for lack of knowledge to the contrary. (The partial pressures of Be(g), BeF_2(g), and Aℓ(g) also are shown on these graphs.) In the case of AℓCℓ and AℓCℓ_2, however, the generating system chosen was trivalent-aluminum chloride vapor and the condensed phase Aℓ. Since only one condensed phase is present in these last two cases, there is in addition to the temperature an extra degree of freedom, and this was taken account of by plotting different curves with the total pressure of trivalent-aluminum chloride ($p_{A\ell C\ell_3} + p_{A\ell_2C\ell_6}$) as the parameter. It is for this reason that the curves have marked curvature, since trivalent-aluminum chloride is an equilibrium mixture of the monomer and dimer which in the pressure range involved varies from nearly all dimer at the lowest temperatures to nearly all monomer at the highest temperatures. While the vapor pressures of trivalent-aluminum chloride are relatively high compared with those of BeF_2 and $A\ell F_3$, it should be noted that for each of the curves of Figs. 3a, 3b, 4a, and 4b the given pressure of this chloride exceeds the vapor pressure below a certain temperature and hence represents a metastable region unattainable in practice. (The vapor pressure of trivalent-aluminum chloride is 10^{-6}, 10^{-2}, and 10^{0} at approximately 315°, 395°, and 450°K respectively [1].) The same results are plotted in Fig. 3b as in Fig. 3a, and in Fig. 4b as in Fig. 4a, but the slightly more complicated ordinate function in the "b" graphs allows a reduced ordinate scale which increases the accuracy in reading the graph.

The sources of the basic data assumed in constructing the various graphs are referenced in Table 1, and the heats of formation assumed are tabulated (in some cases with a tolerance representing the uncertainty given in the reference cited).

Table 1

Sources of Basic Data Used in Constructing Figures 1 to 4(b)
(References to NBS Reports: No. 6928 (1960)[2], No. 7437 (1962)[3])

Substance and State	ΔHf^o_0 Assumed	Equivalent ΔH^o_0 to Gaseous Atoms	Reference to ΔHf^o_0 Assumed	Reference to Free-Energy Functions Assumed
	kcal/mole	kcal/mole		
Be(c,ℓ)	0	76.8_9	[2],p.C-2	[2], Table B-7
Be(g)	$+76.8_9$	0	[2],p.C-2	[2], Table A-4
BeF(g)	$+3._{24}$ ±30	92. ±30	[2],p.C-4	[2], Table A-23
	-29.2_6	124.5	Herzberg [4]	
	-89.2_6	184.5	[5]	
BeF_2(c,ℓ)	-239.9_2 ±2	353.5_2	[2],p.C-4,for ΔHf^o_{298}	[3], Table B-58
BeF_2(g)	-182.5_5 ±6	296.1_5 ±6	[2],p.C-4	[2], Table A-51
Aℓ(c,ℓ)	0	76.9_4	[2],p.C-2	[2], Table B-1
Aℓ(g)	$+76.9_4$	0	[2],p.C-2	[2], Table A-13
AℓF(g)	-49.2	144.5	Hypothetical; see text.	[2], Table A-31
	-61.2_8 ±2	156.5_8 ±2	[2],p.C-3	
	-71.4	166.7	Hypothetical	
$A\ell F_3$(c)	-357.0 ±2	487.5	[3], p.41	[2], Table B-5
AℓCℓ(g)	-11.3_4 ±1	116.8_2 ±1	[2],p.C-3	[2], Table A-32
$A\ell C\ell_2$(g)	-77.8_1 ±5	211.8_3 ±5	[2],p.C-3	[2], Table A-67
$A\ell C\ell_3$(g)	-138.4_8 ±2	301.0_4 ±2	[2],p.C-3	[2], Table A-68
$A\ell_2C\ell_6$(g)	-311.3_9 ±2	636.5_1 ±2	[2],p.C-4	[2], Table A-69

In those cases where two or more values for a standard heat of formation (or dissociation energy) which differ by more than 5 kcal/mole are seriously proposed by different authors, a separate curve is given based on each. It should be emphasized, however, that in the present chapter no claim is made to having necessarily selected the best values for the heats of formation nor to having assessed the probable uncertainties of the values used. Reference may be made to the previous reports from this program [6] for the reasons for making there specific selections among conflicting values reported. In the case of the standard heat of formation of BeF, at least three widely different values have been proposed, and a critical discussion of the evidence is given in the preceding chapter (B-8) of the present report. For $A\ell F(g)$, the values currently proposed are close to $\Delta Hf_0^o = -61$ kcal/mole. A recent investigator [7] calculated from his data a heat of formation corresponding to $\Delta Hf_0^o = -50.9$ kcal/mole, but we traced the discrepancy of this value to his having used an old value of approximately $\Delta Hf_0^o = -320$ kcal/mole for $A\ell F_3(c)$ (cf. Chap. B-1). (Gross et al had derived $\Delta Hf_0^o = -49$ kcal/mole for $A\ell F(g)$ in 1948 [8], but revised their value to -59.2 in 1954 [9].) Hence the highest and lowest curves in Fig. 2 are based on hypothetical heats of formation of $A\ell F$, but serve to indicate the effect of uncertainty in this constant.

The standard heat of formation of $A\ell C\ell(g)$ seems to be rather accurately established. The value for $A\ell C\ell_2(g)$ may have a larger uncertainty than that estimated (see Table 1). However the displacement of any curve in Figs. 4(a) and 4(b) (or in fact for any gas) when one assumes a different value for its dissociation energy can readily be calculated from the relation.

$$\delta \log p = -218.5 \, (\delta \Delta Hf_0^o)/T = 218.5 \, (\delta \Delta H_0)/T,$$

where ΔHf_0^o and ΔH_0 are, in kcal/mole, the standard heat of formation and the dissociation energy respectively of the gas.

References

1. NBS Report 6484, National Bureau of Standards, Washington, D. C., 1 July 1959, pp. 69-70.

2. NBS Report 6928, National Bureau of Standards, Washington, D. C., 1 July 1960.

3. NBS Report 7437, National Bureau of Standards, Washington, D. C., 1 January 1962.

4. G. Herzberg, "Molecular Spectra and Molecular Structure: I. Diatomic Molecules," 2nd Edition, Prentice-Hall, Inc., New York, N.Y., 1950.

5. V. M. Tatevskii, L. N. Tunitskii, and M. M. Novikov, "Vibrational Constants and Dissociation Energy of the BeF Molecule," Optika i Spektroskopiya 5, 520-529 (1958); cf. Chem. Abstr. 53, 2774c (1959).

6. NBS Reports (National Bureau of Standards, Washington, D. C.): No. 6297 (1 Jan. 1959), pp. 36-46, 57-68; No. 6484 (1 July 1959), pp. 45-48, 66-71, 82-92; No. 6645 (1 Jan. 1960), pp. 65-66; No. 6928 (1 July 1960), pp. C-1 to C-4; No. 7093 (1 Jan. 1961), p. 169; No. 7192 (1 July 1961), pp. 101-103, 111-114; No. 7437 (1 Jan. 1962), pp. 40-42, 48.

7. S. A. Semenkovich, Trudy Vsesoyuz. Alyumin.-Magnievyi Inst. 1960, No. 44, 113-119 (1960); cf. Chem. Abstr. 55, 17326g (1961).

8. P. Gross, C. S. Campbell, P. J. C. Kent, and D. L. Levi, Discussions Faraday Soc. 1948, No. 4, 206-215 (1948).

9. P. Gross, C. Hayman, and D. L. Levi, Trans. Faraday Soc. 50, 477-480 (1954).

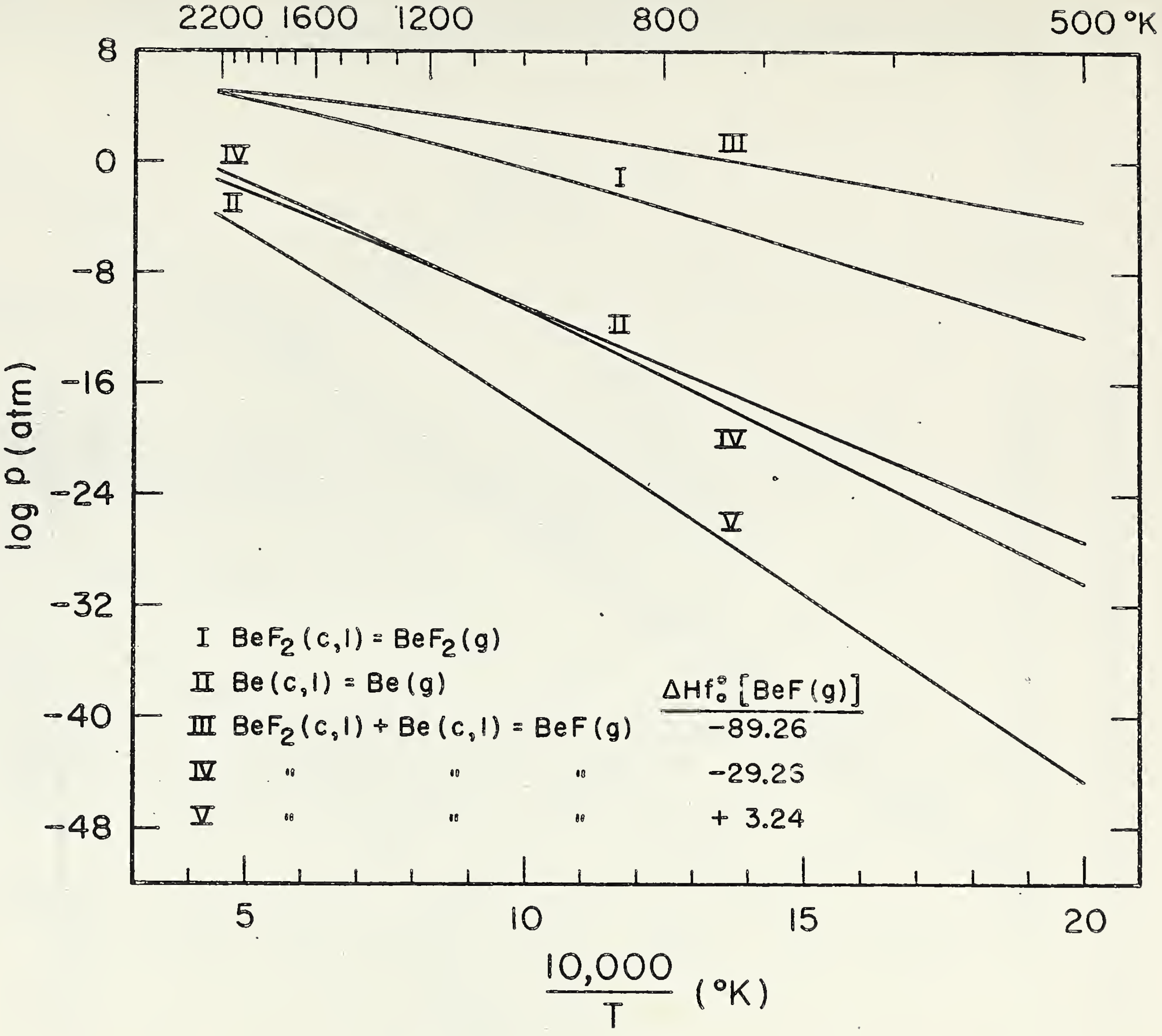


Fig. 1. Pressures of BeF(g), BeF_2(g), and Be(g) in Equilibrium with Condensed BeF_2 and Condensed Be

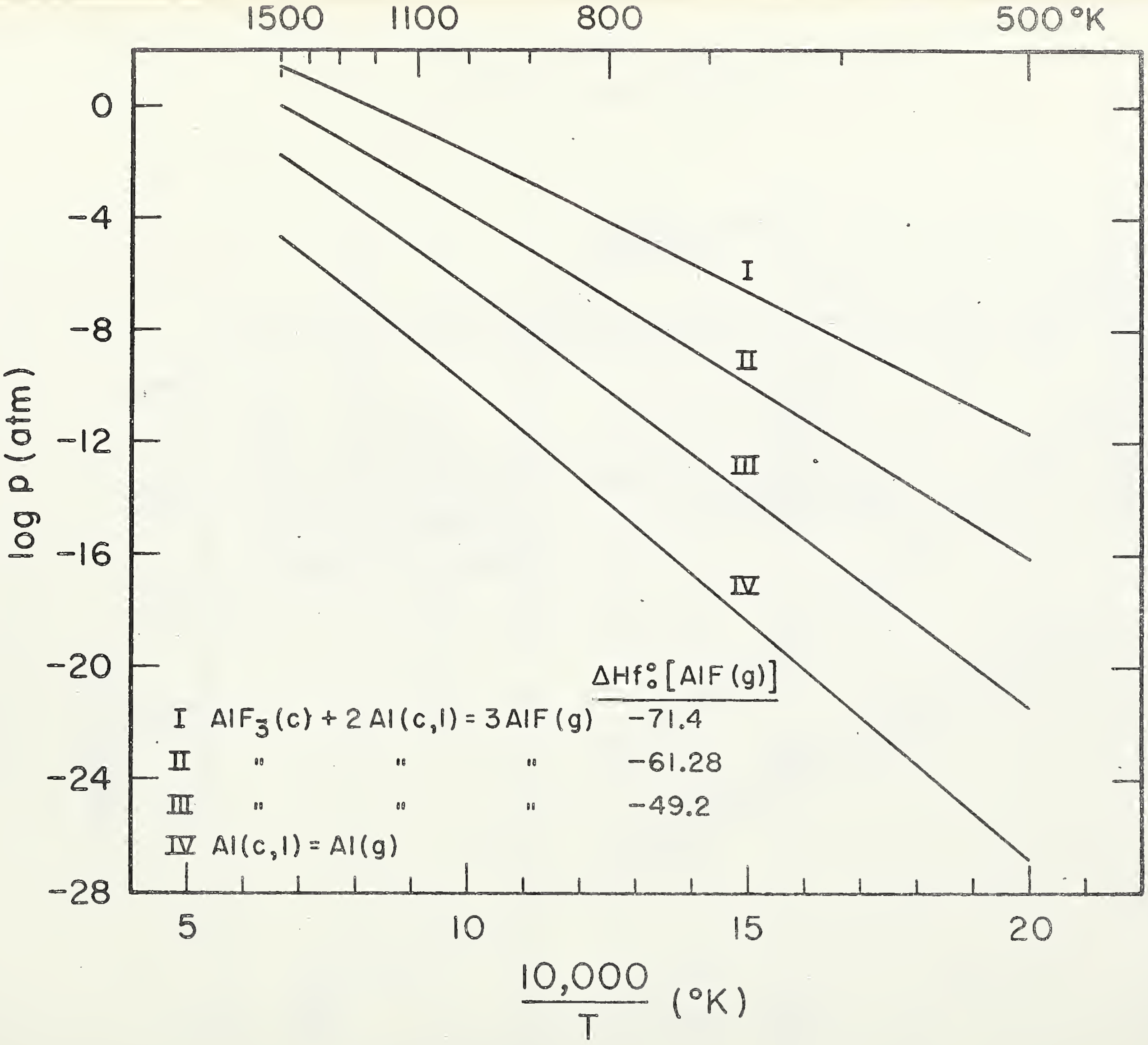


Fig. 2. Pressures of $AlF(g)$ and $Al(g)$ in Equilibrium with Condensed AlF_3 and Condensed Al

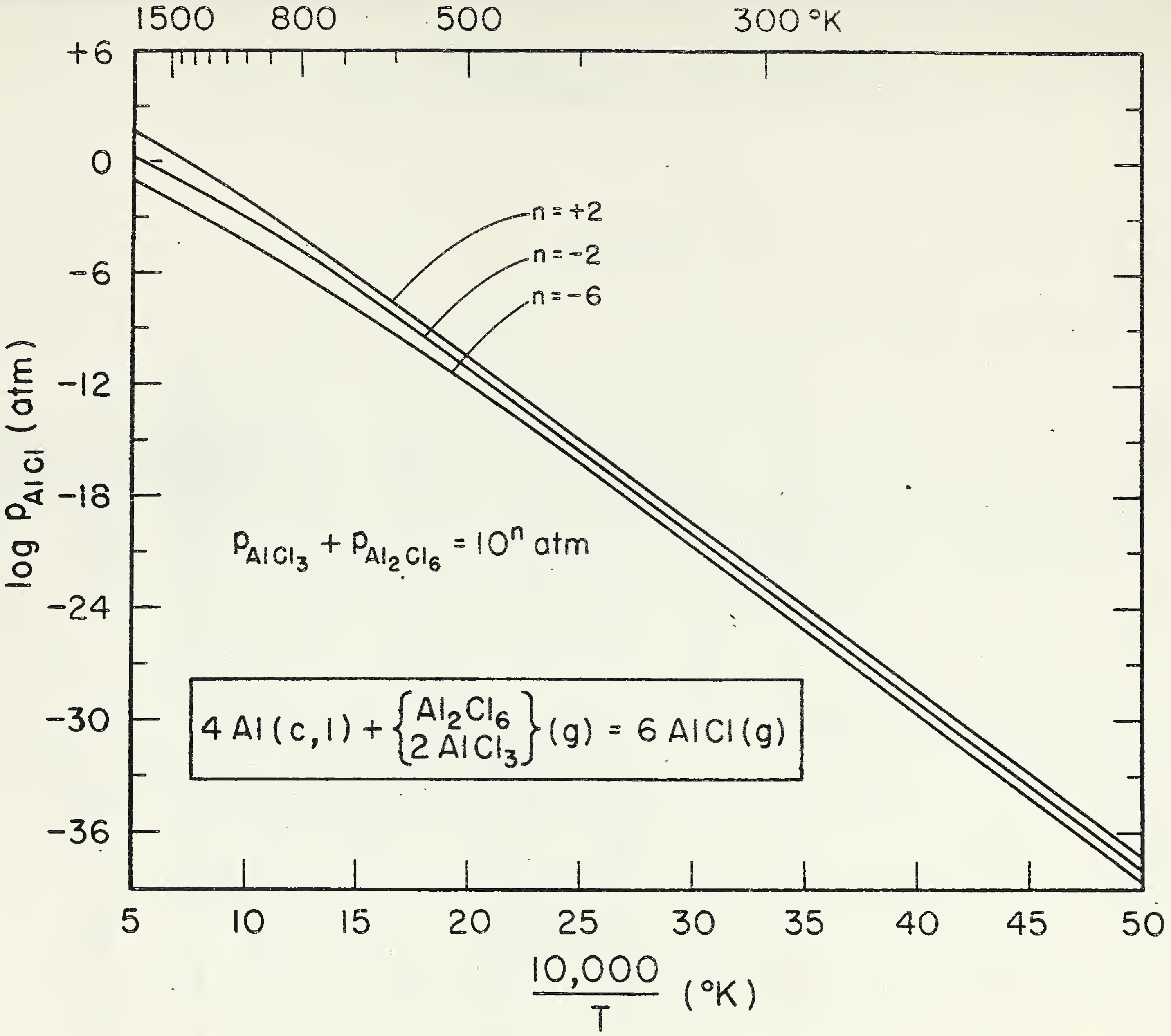


Fig. 3a. Pressures of $AlCl(g)$ in Equilibrium with Gaseous Aluminum Chloride and Condensed Al

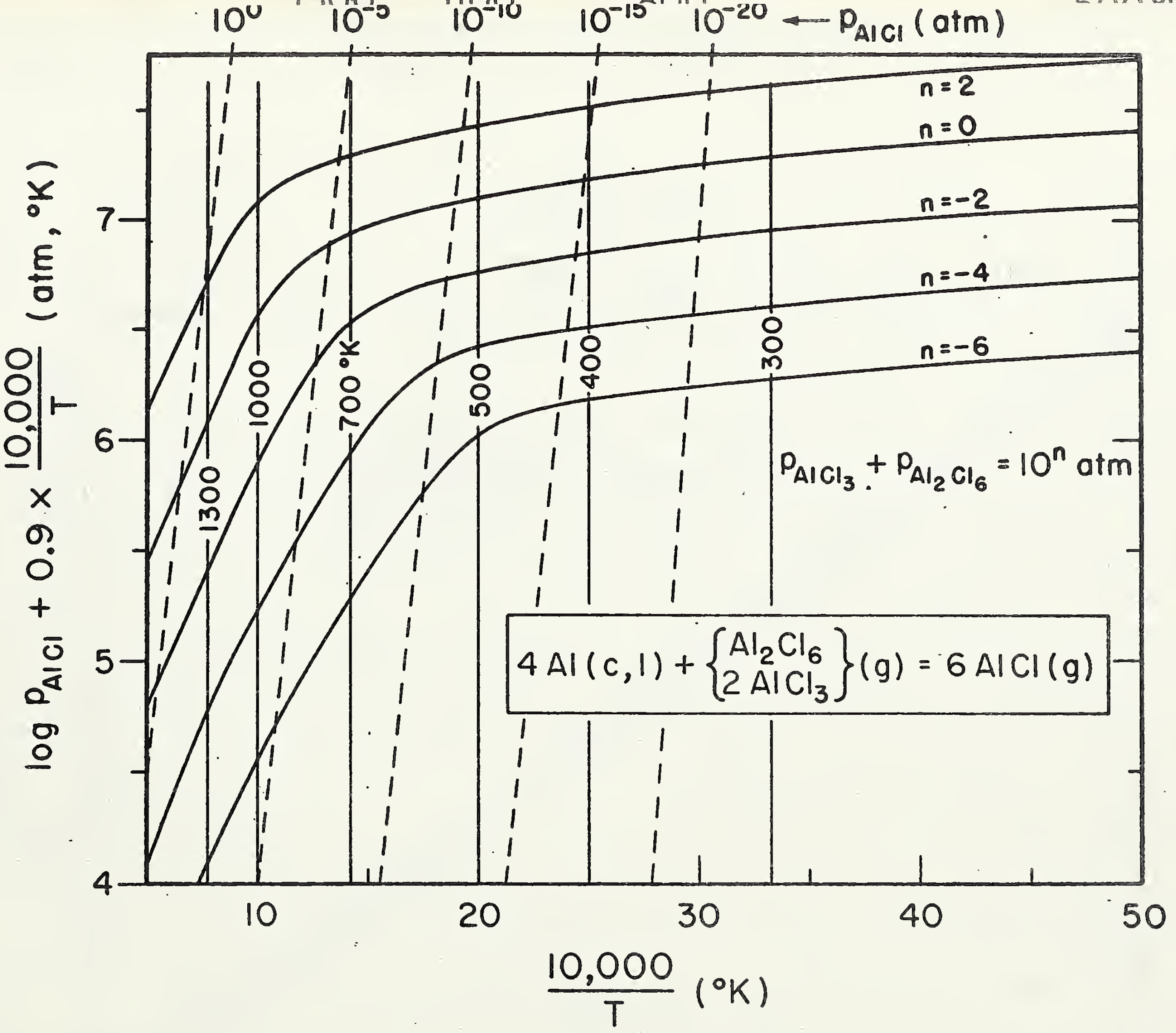


Fig. 3b. Pressures of $AlCl(g)$ in Equilibrium with Gaseous Aluminum Chloride and Condensed Al

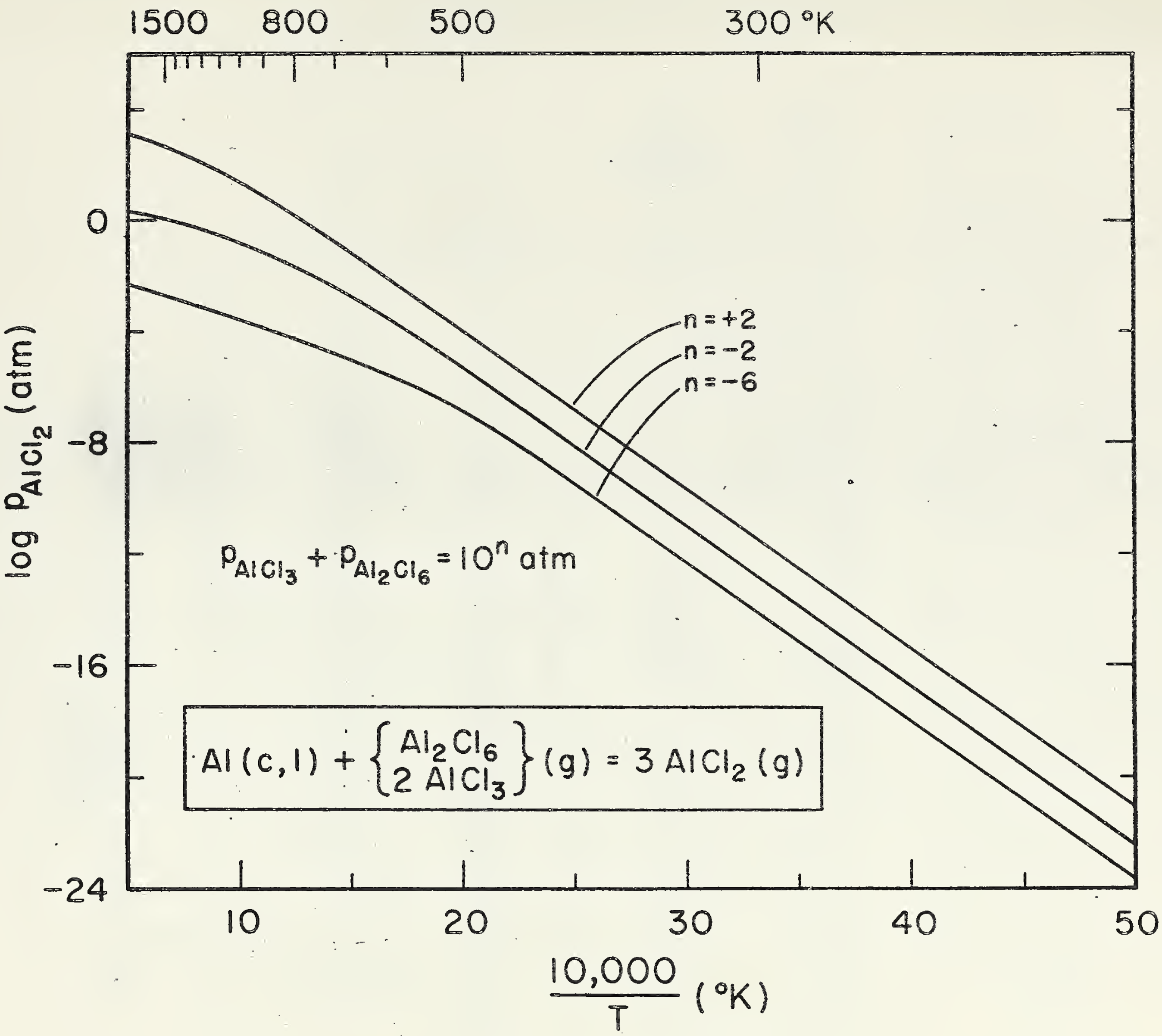


Fig. 4a. Pressures of $A\ell C\ell_2(g)$ in Equilibrium with Gaseous Aluminum Chloride and Condensed $A\ell$

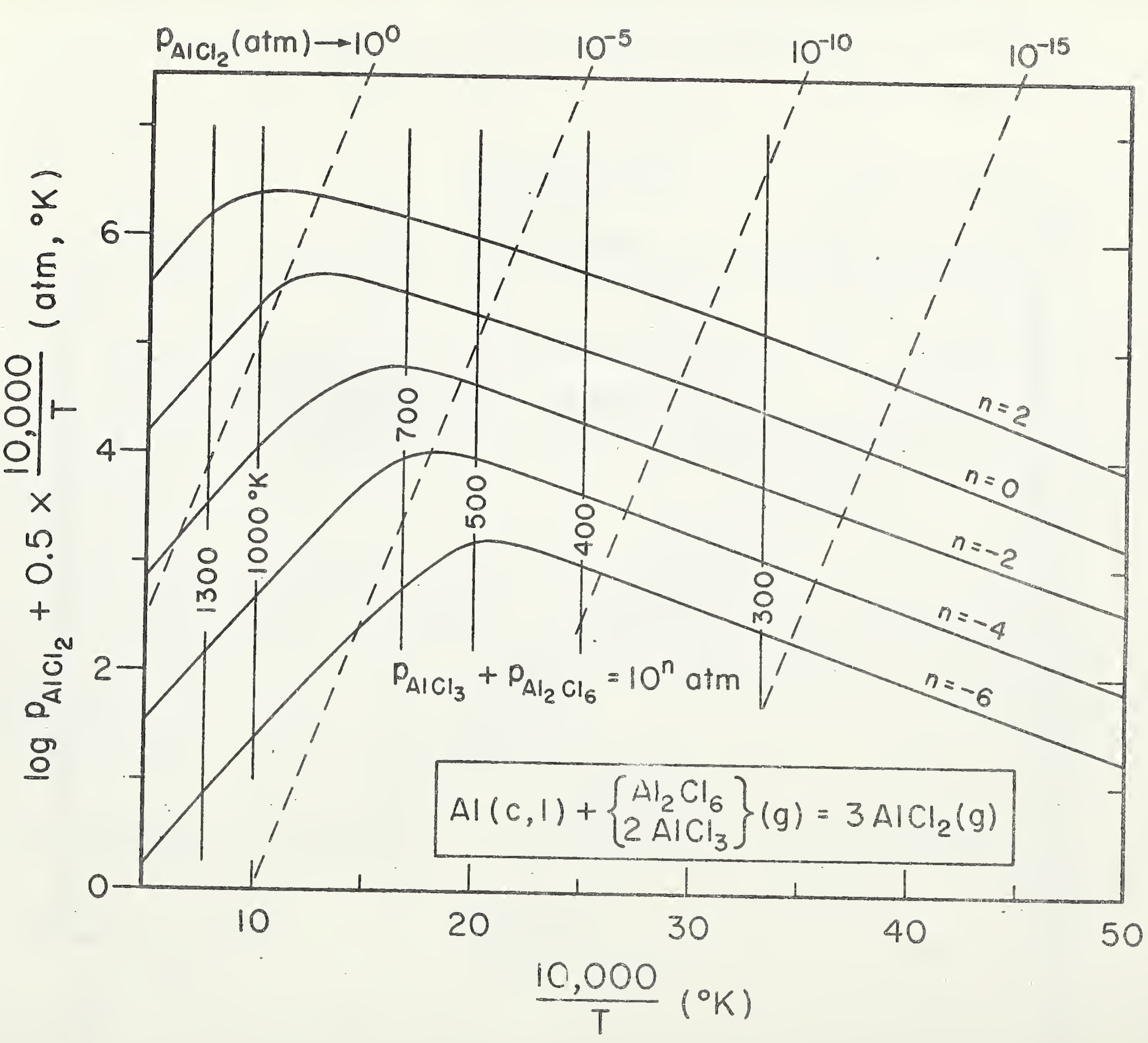


Fig. 4b. Pressures of $AlCl_2(g)$ in Equilibrium with Gaseous Aluminum Chloride and Condensed Al

Chapter B-10

THERMODYNAMIC FUNCTIONS OF DIFLUORAMINE

by D. E. Mann and D. R. Lide, Jr.

The pure rotational spectrum of difluoramine has been studied with a Stark-modulation microwave spectrometer [1]. The spectrum follows a rigid asymmetric rotor pattern with no resolvable inversion doubling. The analysis gives the following rotational constants for NF_2H: A = 1.76846 cm^{-1}, B = 3.63430 cm^{-1}, and C = 3.10450 cm^{-1}. A similar analysis of the NF_2D spectrum gives: A = 1.49720 cm^{-1}, B = 3.58560 cm^{-1}, and C = 3.04420 cm^{-1}.

The infrared vibrational spectra of gaseous NF_2H and NF_2D have been investigated with a Beckman lR-T spectrometer [2]. The fundamentals for the former are: 3193, 1424, 1307, 972, 888, and 500 cm^{-1}; while for the latter they are 2333 (estimated), 1042, 1008, 972, 888, and 500 (estimated).

Ideal-gas thermodynamic functions for NF_2H and NF_2D based on the above molecular constants have been computed up to 6000°K by an IBM 7090 digital computer, and are given in Appendix A as Tables A-84 and A-85 respectively.

References

1. D. R. Lide, Jr., NBS Report 7553, Microwave Spectrum and Structure of Difluoramine, National Bureau of Standards, Washington, D. C., July 1962.

2. J. J. Comeford, D. E. Mann, L. J. Schoen, and D. R. Lide, Jr., NBS Report 7554, Infrared Spectrum of Difluoramine, National Bureau of Standards, Washington, D. C., August 1962.

APPENDIX A

IDEAL-GAS THERMODYNAMIC FUNCTIONS

(For a relevant discussion, see Chapter B-10.)

Table A-84 Thermodynamic Functions for NF_2H

T °K	$-(F^o-H^o_0)/T$	$(H^o-H^o_0)/T$	S^o	C^o_p	$(H^o-H^o_0)$	$-(F^o-H^o_{298.15})/T$
273.15	50.981	8.523	59.505	9.983	2328.1	60.436
298.15	51.734	8.662	60.395	10.366	2582.5	60.395
50.	37.308	7.943	45.251	7.949	397.1	88.957
75.	40.529	7.946	48.475	7.961	596.0	74.962
100.	42.816	7.957	50.772	8.027	795.7	68.641
125.	44.594	7.984	52.578	8.170	998.0	65.254
150.	46.053	8.031	54.085	8.378	1204.7	63.270
175.	47.296	8.099	55.395	8.639	1417.3	62.053
200.	48.383	8.185	56.568	8.942	1637.0	61.296
225.	49.353	8.287	57.640	9.277	1864.7	60.831
250.	50.232	8.404	58.636	9.636	2101.0	60.562
275.	51.039	8.533	59.572	10.011	2346.6	60.430
300.	51.787	8.672	60.460	10.395	2601.7	60.396
325.	52.487	8.820	61.307	10.779	2866.4	60.433
350.	53.147	8.973	62.120	11.159	3140.6	60.525
375.	53.771	9.131	62.902	11.530	3424.2	60.658
400.	54.365	9.292	63.658	11.887	3717.0	60.822
425.	54.934	9.455	64.389	12.230	4018.5	61.010
450.	55.479	9.619	65.097	12.557	4328.4	61.218
475.	56.003	9.782	65.785	12.868	4646.2	61.440
500.	56.509	9.943	66.452	13.161	4971.6	61.674
550.	57.472	10.261	67.732	13.701	5643.4	62.167
600.	58.378	10.568	68.946	14.181	6340.7	62.682
650.	59.235	10.862	70.098	14.608	7060.6	63.208
700.	60.051	11.144	71.195	14.990	7800.7	63.740
750.	60.829	11.412	72.241	15.333	8559.0	64.272
800.	61.573	11.667	73.240	15.643	9333.5	64.802
850.	62.288	11.909	74.197	15.923	10122.8	65.326
900.	62.975	12.139	75.115	16.178	10925.4	65.845
950.	63.638	12.358	75.996	16.411	11740.3	66.356
1000.	64.277	12.566	76.843	16.624	12566.2	66.859
1050.	64.895	12.764	77.659	16.820	13402.4	67.354
1100.	65.493	12.953	78.446	17.000	14248.0	67.841
1150.	66.073	13.132	79.205	17.166	15102.1	68.318
1200.	66.635	13.304	79.939	17.319	15964.3	68.787
1250.	67.182	13.467	80.649	17.461	16833.8	69.248
1300.	67.713	13.623	81.336	17.592	17710.2	69.699
1350.	68.230	13.772	82.002	17.713	18592.9	70.143
1400.	68.733	13.915	82.649	17.826	19481.4	70.578
1450.	69.224	14.052	83.276	17.931	20375.4	71.005
1500.	69.703	14.183	83.886	18.029	21274.4	71.424
1550.	70.170	14.308	84.478	18.120	22178.2	71.836
1600.	70.626	14.429	85.055	18.205	23086.3	72.240
1650.	71.072	14.545	85.616	18.285	23998.6	72.637
1700.	71.508	14.656	86.163	18.359	24914.7	73.027
1750.	71.934	14.763	86.697	18.428	25834.4	73.410
1800.	72.351	14.865	87.217	18.493	26757.5	73.786

Table A-84 Thermodynamic Functions for NF_2H - Continued

T °K	$\frac{-(F^o-H^o_0)}{T}$	$\frac{(H^o-H^o_0)}{T}$	S^o	C^o_p	$(H^o-H^o_0)$	$\frac{-(F^o-H^o_{298.15})}{T}$
1850.	72.760	14.964	87.724	18.554	27683.7	74.156
1900.	73.160	15.059	88.220	18.612	28612.8	74.520
1950.	73.553	15.151	88.704	18.665	29544.8	74.877
2000.	73.937	15.240	89.177	18.716	30479.3	75.229
2050.	74.315	15.325	89.640	18.764	31416.3	75.575
2100.	74.685	15.407	90.093	18.809	32355.6	75.915
2150.	75.049	15.487	90.536	18.851	33297.1	76.250
2200.	75.406	15.564	90.969	18.891	34240.7	76.579
2250.	75.756	15.638	91.394	18.929	35186.2	76.904
2300.	76.101	15.710	91.811	18.965	36133.5	77.223
2350.	76.439	15.780	92.219	18.998	37082.6	77.538
2400.	76.772	15.847	92.619	19.030	38033.3	77.848
2450.	77.100	15.913	93.012	19.061	38985.6	78.154
2500.	77.422	15.976	93.397	19.090	39939.4	78.455
2600.	78.051	16.097	94.147	19.143	41851.1	79.044
2700.	78.660	16.210	94.871	19.191	43767.8	79.617
2800.	79.252	16.318	95.569	19.235	45689.1	80.174
2900.	79.826	16.419	96.245	19.275	47614.6	80.717
3000.	80.384	16.515	96.899	19.311	49543.9	81.245
3100.	80.927	16.605	97.533	19.344	51476.7	81.761
3200.	81.456	16.691	98.147	19.374	53412.6	82.263
3300.	81.971	16.773	98.744	19.402	55351.5	82.753
3400.	82.473	16.851	99.324	19.428	57293.0	83.232
3500.	82.962	16.925	99.887	19.451	59237.0	83.700
3600.	83.440	16.995	100.435	19.473	61183.2	84.157
3700.	83.907	17.063	100.969	19.493	63131.5	84.605
3800.	84.363	17.127	101.489	19.512	65081.8	85.042
3900.	84.808	17.188	101.996	19.529	67033.9	85.470
4000.	85.244	17.247	102.491	19.546	68987.7	85.890
4100.	85.671	17.303	102.974	19.561	70943.0	86.301
4200.	86.088	17.357	103.445	19.575	72899.8	86.703
4300.	86.497	17.409	103.906	19.588	74857.9	87.098
4400.	86.898	17.458	104.357	19.600	76817.3	87.485
4500.	87.291	17.506	104.797	19.612	78777.9	87.865
4600.	87.676	17.552	105.228	19.622	80739.6	88.238
4700.	88.054	17.596	105.651	19.633	82702.4	88.604
4800.	88.425	17.639	106.064	19.642	84666.1	88.963
4900.	88.789	17.680	106.469	19.651	86630.8	89.316
5000.	89.147	17.719	106.866	19.660	88596.3	89.663
5100.	89.498	17.757	107.256	19.668	90562.7	90.005
5200.	89.843	17.794	107.638	19.675	92529.9	90.340
5300.	90.183	17.830	108.012	19.682	94497.7	90.670
5400.	90.516	17.864	108.380	19.689	96466.3	90.994
5500.	90.844	17.897	108.742	19.696	98435.6	91.314
5600.	91.167	17.930	109.097	19.702	100405.4	91.628
5700.	91.485	17.961	109.445	19.707	102375.9	91.938
5800.	91.797	17.991	109.788	19.713	104346.9	92.243
5900.	92.105	18.020	110.125	19.718	106318.5	92.543
6000.	92.408	18.048	110.457	19.723	108290.5	92.839

```
  MOLECULAR WEIGHT    53.0115 ROTATIONAL SYMMETRY    1
 ELECTRONIC MULTIPLICITY    1  STRETCHING CONSTANT  0.
  ROTATIONAL CONSTANTS, CM-1
 A  1.7684600E 00    B  3.6343000E-01    C  3.1045000E-01
  FREQUENCY DEGENERACY   FREQUENCY DEGENERACY   FREQUENCY DEGENERACY
  3193.0000        1      1424.0000       1      1307.0000        1
   972.0000        1       888.0000       1       500.0000        1
```

Table A-85 Thermodynamic Functions for NF_2D

T °K	$\frac{-(F^o-H^o_0)}{T}$	$\frac{(H^o-H^o_0)}{T}$	S^o	C^o_p	$(H^o-H^o_0)$	$-(F^o-H^o_{298.15})$
273.15	51.251	8.599	59.850	10.355	2348.8	60.819
298.15	52.011	8.766	60.777	10.829	2613.6	60.777
50.	37.562	7.943	45.505	7.949	397.1	89.833
75.	40.783	7.946	48.729	7.961	596.0	75.631
100.	43.070	7.957	51.027	8.028	795.7	69.206
125.	44.848	7.984	52.832	8.174	998.0	65.757
150.	46.308	8.033	54.341	8.398	1205.0	63.732
175.	47.551	8.106	55.657	8.694	1418.5	62.486
200.	48.640	8.201	56.841	9.056	1640.3	61.708
225.	49.612	8.319	57.931	9.470	1871.7	61.228
250.	50.496	8.456	58.952	9.921	2114.1	60.950
275.	51.309	8.611	59.920	10.390	2367.9	60.813
300.	52.065	8.779	60.844	10.864	2633.6	60.777
325.	52.775	8.957	61.732	11.331	2911.1	60.817
350.	53.445	9.143	62.588	11.782	3200.0	60.913
375.	54.083	9.333	63.416	12.212	3500.0	61.052
400.	54.691	9.526	64.217	12.620	3810.5	61.225
425.	55.275	9.720	64.994	13.003	4130.8	61.424
450.	55.836	9.912	65.748	13.362	4460.4	61.644
475.	56.377	10.102	66.479	13.698	4798.7	61.879
500.	56.900	10.290	67.190	14.011	5145.1	62.127
550.	57.898	10.655	68.552	14.578	5860.1	62.650
600.	58.840	11.003	69.843	15.073	6601.7	63.196
650.	59.734	11.333	71.067	15.508	7366.5	63.754
700.	60.585	11.645	72.230	15.891	8151.6	64.319
750.	61.399	11.940	73.338	16.230	8954.8	64.883
800.	62.178	12.217	74.396	16.531	9774.0	65.445
850.	62.927	12.479	75.406	16.799	10607.4	66.001
900.	63.647	12.726	76.373	17.038	11453.4	66.551
950.	64.341	12.959	77.300	17.253	12310.8	67.093
1000.	65.012	13.178	78.190	17.446	13178.4	67.625
1050.	65.660	13.386	79.046	17.620	14055.1	68.149
1100.	66.287	13.582	79.869	17.777	14940.1	68.663
1150.	66.895	13.767	80.662	17.920	15832.6	69.168
1200.	67.485	13.943	81.428	18.049	16731.8	69.663
1250.	68.057	14.110	82.167	18.166	17637.2	70.148
1300.	68.614	14.268	82.882	18.273	18548.3	70.624
1350.	69.155	14.418	83.573	18.371	19464.4	71.091
1400.	69.682	14.561	84.243	18.461	20385.2	71.549
1450.	70.195	14.697	84.892	18.543	21310.3	71.998
1500.	70.696	14.826	85.522	18.618	22239.4	72.438
1550.	71.184	14.950	86.134	18.688	23172.1	72.870
1600.	71.660	15.068	86.728	18.752	24108.1	73.294
1650.	72.126	15.180	87.306	18.811	25047.2	73.710
1700.	72.581	15.288	87.868	18.866	25989.1	74.118
1750.	73.025	15.391	88.416	18.917	26933.7	74.519
1800.	73.460	15.489	88.950	18.964	27880.7	74.912

Table A-85 Thermodynamic Functions for NF_2D - Continued

T °K	$\frac{-(F^o-H^o_0)}{T}$	$\frac{(H^o-H^o_0)}{T}$	S^o	C^o_p	$(H^o-H^o_0)$	$\frac{-(F-H^o_{298.15})}{T}$
1850.	73.886	15.584	89.470	19.008	28830.0	75.299
1900.	74.303	15.674	89.977	19.049	29781.5	75.678
1950.	74.711	15.761	90.472	19.087	30734.8	76.051
2000.	75.111	15.845	90.956	19.122	31690.1	76.418
2050.	75.503	15.925	91.429	19.156	32647.0	76.778
2100.	75.888	16.003	91.891	19.187	33605.6	77.133
2150.	76.265	16.077	92.343	19.216	34565.7	77.481
2200.	76.636	16.149	92.785	19.244	35527.2	77.824
2250.	77.000	16.218	93.217	19.269	36490.0	78.161
2300.	77.357	16.284	93.641	19.294	37454.1	78.493
2350.	77.708	16.349	94.056	19.316	38419.4	78.820
2400.	78.053	16.411	94.463	19.338	39385.7	79.142
2450.	78.392	16.471	94.862	19.358	40353.1	79.458
2500.	78.725	16.529	95.253	19.378	41321.5	79.770
2600.	79.375	16.639	96.014	19.413	43261.1	80.381
2700.	80.005	16.742	96.747	19.445	45204.0	80.973
2800.	80.616	16.839	97.455	19.473	47150.0	81.549
2900.	81.208	16.931	98.139	19.499	49098.6	82.110
3000.	81.784	17.017	98.800	19.523	51049.7	82.655
3100.	82.343	17.098	99.441	19.544	53003.1	83.186
3200.	82.887	17.175	100.062	19.564	54958.5	83.704
3300.	83.417	17.247	100.664	19.581	56915.8	84.209
3400.	83.933	17.316	101.249	19.598	58874.7	84.701
3500.	84.436	17.382	101.817	19.613	60835.3	85.182
3600.	84.926	17.444	102.370	19.627	62797.2	85.652
3700.	85.405	17.503	102.908	19.639	64760.5	86.111
3800.	85.872	17.559	103.432	19.651	66725.1	86.560
3900.	86.329	17.613	103.942	19.662	68690.7	86.999
4000.	86.776	17.664	104.440	19.672	70657.4	87.429
4100.	87.213	17.713	104.926	19.681	72625.1	87.850
4200.	87.640	17.760	105.400	19.690	74593.7	88.262
4300.	88.058	17.805	105.864	19.698	76563.1	88.666
4400.	88.468	17.848	106.317	19.706	78533.4	89.062
4500.	88.870	17.890	106.760	19.713	80504.3	89.451
4600.	89.264	17.930	107.193	19.720	82476.0	89.832
4700.	89.650	17.968	107.617	19.726	84448.3	90.206
4800.	90.028	18.004	108.033	19.732	86421.2	90.573
4900.	90.400	18.040	108.440	19.738	88394.7	90.933
5000.	90.765	18.074	108.838	19.743	90368.7	91.287
5100.	91.123	18.107	109.229	19.748	92343.3	91.635
5200.	91.475	18.138	109.613	19.753	94318.3	91.977
5300.	91.821	18.169	109.989	19.757	96293.8	92.314
5400.	92.160	18.198	110.358	19.761	98269.7	92.644
5500.	92.495	18.227	110.721	19.765	100246.0	92.970
5600.	92.823	18.254	111.077	19.769	102222.7	93.290
5700.	93.147	18.281	111.427	19.772	104199.7	93.605
5800.	93.465	18.306	111.771	19.776	106177.1	93.915
5900.	93.778	18.331	112.109	19.779	108154.8	94.221
6000.	94.086	18.355	112.442	19.782	110132.9	94.522

APPENDIX B

THERMODYNAMIC FUNCTIONS FOR SOLIDS AND LIQUIDS

(For relevant discussions, see Chapters B-2, B-3, and B-7.)

TABLE B-29 REVISED

THERMODYNAMIC FUNCTIONS FOR BERYLLIUM NITRIDE (Be_3N_2)

SOLID AND LIQUID PHASES

GRAM MOLECULAR WEIGHT = 55.040 GRAMS 1 CAL = 4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$[-(G^{o}_{T}-H^{o}_{298})/T]-S^{o}_{298}$ CAL/DEG MOLE	$(H^{o}_{T}-H^{o}_{298})/T$ CAL/DEG MOLE	$(S^{o}_{T}-S^{o}_{298})$ CAL/DEG MOLE	$(H^{o}_{T}-H^{o}_{298})$ CAL/MOLE	C^{o}_{P} CAL/DEG MOLE	$[-(G^{o}_{T}-H^{o}_{298})-TS^{o}_{298}]$ CAL/MOLE
			(SOLID)			
298.15	0.000	0.000	0.000	0.000	15.405	0.000
300.00	0.000	0.095	0.096	28.576	15.488	0.088
310.00	0.012	0.599	0.611	185.78	15.957	3.622
320.00	0.038	1.087	1.125	347.77	16.443	12.304
330.00	0.079	1.560	1.639	514.66	16.934	26.125
340.00	0.133	2.019	2.152	686.46	17.425	45.077
350.00	0.198	2.466	2.664	863.14	17.910	69.154
360.00	0.273	2.902	3.175	1044.6	18.384	98.348
370.00	0.359	3.326	3.685	1230.8	18.845	132.65
373.15	0.387	3.458	3.845	1290.4	18.987	144.51
380.00	0.453	3.741	4.193	1421.5	19.292	172.04
390.00	0.555	4.145	4.700	1616.6	19.722	216.51
400.00	0.665	4.540	5.205	1815.9	20.137	266.04
425.00	0.969	5.486	6.455	2331.5	21.100	411.82
450.00	1.308	6.378	7.686	2870.0	21.963	588.62
475.00	1.676	7.219	8.894	3428.9	22.733	795.93
500.00	2.066	8.012	10.078	4006.0	23.420	1033.1
550.00	2.899	9.468	12.367	5207.1	24.583	1594.7
600.00	3.780	10.768	14.548	6460.6	25.523	2268.0
650.00	4.689	11.933	16.622	7756.7	26.296	3047.7
700.00	5.612	12.983	18.595	9088.2	26.945	3928.6
750.00	6.541	13.933	20.474	10450.	27.501	4905.7
800.00	7.468	14.796	22.264	11837.	27.988	5974.5
850.00	8.389	15.585	23.974	13248.	28.423	7130.8
900.00	9.301	16.310	25.611	14679.	28.820	8370.7
950.00	10.201	16.978	27.179	16129.	29.188	9690.7
1000.00	11.088	17.597	28.685	17597.	29.534	11088.
1050.00	11.960	18.173	30.134	19082.	29.864	12558.
1100.00	12.818	18.712	31.530	20583.	30.182	14100.
1150.00	13.661	19.218	32.879	22100.	30.491	15710.
1200.00	14.489	19.694	34.183	23632.	30.795	17387.
1250.00	15.302	20.144	35.446	25180.	31.094	19128.
1300.00	16.101	20.571	36.671	26742.	31.390	20931.
1350.00	16.885	20.977	37.862	28319.	31.685	22795.
1400.00	17.655	21.364	39.019	29910.	31.979	24717.
1450.00	18.411	21.736	40.147	31516.	32.273	26696.
1500.00	19.154	22.092	41.246	33137.	32.567	28731.
1550.00	19.884	22.434	42.318	34773.	32.863	30820.
1600.00	20.601	22.765	43.366	36424.	33.159	32962.
1650.00	21.307	23.084	44.391	38089.	33.457	35156.
1700.00	22.001	23.394	45.394	39769.	33.756	37401.
1750.00	22.683	23.694	46.377	41465.	34.057	39695.
1800.00	23.355	23.986	47.341	43175.	34.360	42039.
1850.00	24.016	24.271	48.287	44901.	34.665	44429.
1900.00	24.667	24.548	49.215	46642.	34.972	46867.
1950.00	25.308	24.820	50.127	48398.	35.280	49351.
2000.00	25.940	25.085	51.025	50170.	35.590	51879.
2050.00	26.562	25.345	51.907	51957.	35.903	54453.
2100.00	27.176	25.600	52.776	53760.	36.217	57070.
2150.00	27.781	25.851	53.632	55579.	36.532	59730.
2200.00	28.379	26.097	54.476	57413.	36.850	62433.
2250.00	28.968	26.339	55.307	59264.	37.169	65177.
2300.00	29.549	26.578	56.128	61130.	37.490	67963.
2350.00	30.123	26.814	56.937	63013.	37.812	70790.
2400.00	30.690	27.047	57.737	64912.	38.136	73657.
2450.00	31.250	27.276	58.527	66827.	38.462	76564.
2470.00	31.473	27.367	58.840	67597.	38.593	77737.
			(LIQUID)			
2470.00	31.473	39.863	71.335	98461.	39.006	77737.
2500.00	31.954	39.852	71.805	99629.	38.886	79884.
2600.00	33.516	39.807	73.323	103498.	38.486	87141.
2700.00	35.017	39.751	74.768	107326.	38.086	94546.
2800.00	36.462	39.684	76.146	111115.	37.686	102093.
2900.00	37.853	39.608	77.461	114864.	37.286	109774.
3000.00	39.194	39.524	78.718	118572.	36.887	117583.
3100.00	40.489	39.433	79.921	122241.	36.487	125515.
3200.00	41.739	39.334	81.074	125870.	36.087	133566.
3300.00	42.948	39.230	82.178	129458.	35.687	141728.
3400.00	44.118	39.120	83.237	133007.	35.287	150000.
3500.00	45.250	39.005	84.254	136516.	34.887	158375.
3600.00	46.347	38.885	85.232	139985.	34.487	166849.
3700.00	47.411	38.760	86.171	143413.	34.088	175420.
3800.00	48.443	38.632	87.075	146802.	33.688	184082.
3900.00	49.444	38.500	87.945	150151.	33.288	192833.
4000.00	50.418	38.365	88.782	153460.	32.888	201670.

H^{0}_{298} AND S^{0}_{298} APPLY TO THE REFERENCE STATE OF THE SOLID AT 298.15 DEG K

THIS TABLE SUPERSEDES TABLE B-29 OF NBS REPORT 6928 AND TABLE 2-29 OF NBS REPORT 6645.

REVISED REVISED

TABLE B-59

THERMODYNAMIC FUNCTIONS FOR ALUMINUM CARBIDE (AL_4C_3)
SOLID PHASE

GRAM MOLECULAR WT.=143.9594 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.000	0.001	0.001	0.000
10.00	0.000	0.001	0.002	0.012	0.005	0.004
15.00	0.001	0.004	0.006	0.062	0.017	0.021
20.00	0.003	0.010	0.013	0.195	0.041	0.065
25.00	0.006	0.021	0.027	0.520	0.095	0.162
30.00	0.012	0.040	0.052	1.207	0.188	0.355
35.00	0.020	0.071	0.091	2.486	0.334	0.707
40.00	0.032	0.117	0.149	4.667	0.549	1.299
45.00	0.050	0.180	0.230	8.094	0.833	2.236
50.00	0.073	0.262	0.335	13.106	1.183	3.636
55.00	0.102	0.364	0.467	20.042	1.603	5.628
60.00	0.139	0.487	0.626	29.236	2.083	8.350
65.00	0.184	0.630	0.814	40.956	2.612	11.939
70.00	0.236	0.792	1.028	55.444	3.191	16.532
75.00	0.297	0.972	1.269	72.910	3.801	22.265
80.00	0.366	1.169	1.534	93.495	4.437	29.264
85.00	0.443	1.380	1.823	117.31	5.089	37.648
90.00	0.528	1.605	2.133	144.41	5.753	47.529
95.00	0.621	1.841	2.462	174.85	6.424	59.007
100.00	0.722	2.087	2.808	208.66	7.099	72.175
105.00	0.830	2.341	3.171	245.84	7.776	87.117
110.00	0.945	2.604	3.549	286.42	8.456	103.91
115.00	1.066	2.873	3.939	330.41	9.138	122.62
120.00	1.194	3.148	4.343	377.80	9.819	143.32
125.00	1.329	3.429	4.757	428.60	10.499	166.07
130.00	1.469	3.714	5.182	482.79	11.175	190.92
135.00	1.614	4.002	5.617	540.34	11.843	217.91
140.00	1.765	4.294	6.059	601.21	12.503	247.10
145.00	1.921	4.589	6.509	665.35	13.154	278.51
150.00	2.081	4.885	6.966	732.73	13.795	312.20
155.00	2.246	5.183	7.429	803.29	14.427	348.19
160.00	2.416	5.481	7.897	876.98	15.048	386.50
165.00	2.589	5.780	8.369	953.75	15.658	427.16
170.00	2.766	6.080	8.846	1033.5	16.258	470.20
175.00	2.946	6.379	9.325	1116.3	16.846	515.62
180.00	3.130	6.678	9.808	1202.0	17.424	563.46
185.00	3.317	6.976	10.293	1290.5	17.991	613.71
190.00	3.507	7.273	10.780	1381.9	18.546	666.39
195.00	3.700	7.569	11.269	1476.0	19.090	721.51
200.00	3.895	7.864	11.759	1572.8	19.622	779.08
205.00	4.093	8.157	12.250	1672.2	20.141	839.11
210.00	4.293	8.448	12.742	1774.2	20.649	901.59
215.00	4.495	8.738	13.233	1878.6	21.144	966.52
220.00	4.700	9.025	13.725	1985.6	21.628	1033.9
225.00	4.906	9.311	14.216	2094.9	22.101	1103.8
230.00	5.113	9.594	14.707	2206.6	22.564	1176.1
235.00	5.323	9.875	15.197	2320.5	23.016	1250.8
240.00	5.534	10.153	15.687	2436.7	23.459	1328.1
245.00	5.746	10.429	16.175	2555.1	23.893	1407.7
250.00	5.959	10.703	16.662	2675.6	24.317	1489.8
255.00	6.174	10.974	17.147	2798.3	24.732	1574.3
260.00	6.389	11.242	17.632	2922.9	25.136	1661.3
265.00	6.606	11.508	18.114	3049.6	25.530	1750.6
270.00	6.824	11.771	18.595	3178.2	25.914	1842.4
273.15	6.961	11.936	18.897	3260.2	26.151	1901.5
275.00	7.042	12.032	19.074	3308.7	26.288	1936.6
280.00	7.261	12.290	19.551	3441.1	26.651	2033.1
285.00	7.481	12.545	20.026	3575.2	27.005	2132.1
290.00	7.701	12.797	20.498	3711.1	27.351	2233.4
295.00	7.922	13.047	20.969	3848.7	27.695	2337.1
298.15	8.062	13.202	21.264	3936.3	27.909	2403.6
300.00	8.144	13.294	21.437	3988.1	28.035	2443.1

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

THIS TABLE SUPERSEDES TABLE B-59 OF NBS REPORT 7437 AND TABLE B-37 OF NBS REPORT 6928.

TABLE B-59(CONT.)

THERMODYNAMIC FUNCTIONS FOR ALUMINUM CARBIDE (AL_4C_3)
SOLID PHASE

GRAM MOLECULAR WT.=143.9594 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
300.00	8.144	13.294	21.437	3988.1	28.035	2443.1
310.00	8.587	13.780	22.367	4271.7	28.694	2662.1
320.00	9.032	14.256	23.288	4561.8	29.314	2890.4
330.00	9.478	14.721	24.199	4857.9	29.894	3127.8
340.00	9.925	15.175	25.100	5159.6	30.439	3374.3
350.00	10.371	15.619	25.990	5466.5	30.952	3629.8
360.00	10.817	16.051	26.868	5778.5	31.435	3894.1
370.00	11.262	16.473	27.736	6095.2	31.893	4167.1
373.15	11.403	16.604	28.007	6195.8	32.032	4254.9
380.00	11.707	16.885	28.592	6416.3	32.324	4448.8
390.00	12.151	17.286	29.437	6741.6	32.726	4738.9
400.00	12.594	17.677	30.270	7070.7	33.104	5037.5
425.00	13.694	18.610	32.304	7909.4	33.973	5819.8
450.00	14.782	19.486	34.268	8768.6	34.746	6652.1
475.00	15.858	20.307	36.166	9646.0	35.439	7532.7
500.00	16.920	21.080	38.000	10540.	36.064	8459.9
550.00	18.996	22.493	41.489	12371.	37.145	10448.
600.00	21.009	23.753	44.761	14252.	38.050	12605.
650.00	22.955	24.883	47.838	16174.	38.818	14921.
700.00	24.837	25.902	50.739	18132.	39.479	17386.
750.00	26.656	26.827	53.483	20120.	40.055	19992.
800.00	28.415	27.670	56.085	22136.	40.561	22732.
850.00	30.116	28.442	58.558	24175.	41.010	25599.
900.00	31.762	29.151	60.913	26236.	41.411	28586.
950.00	33.356	29.806	63.162	28316.	41.772	31688.
1000.00	34.900	30.413	65.313	30413.	42.099	34900.
1050.00	36.398	30.976	67.374	32525.	42.396	38218.
1100.00	37.851	31.502	69.353	34652.	42.669	41636.
1150.00	39.263	31.993	71.255	36792.	42.919	45152.
1200.00	40.634	32.453	73.087	38944.	43.150	48761.
1250.00	41.968	32.885	74.853	41106.	43.364	52460.
1300.00	43.265	33.292	76.557	43280.	43.563	56245.
1350.00	44.529	33.676	78.205	45463.	43.748	60114.
1400.00	45.760	34.039	79.799	47654.	43.922	64065.
1450.00	46.961	34.382	81.343	49855.	44.085	68093.
1500.00	48.132	34.708	82.841	52063.	44.239	72198.
1550.00	49.275	35.018	84.294	54278.	44.384	76377.
1600.00	50.392	35.313	85.705	56501.	44.521	80627.
1650.00	51.483	35.594	87.077	58730.	44.651	84947.
1700.00	52.549	35.862	88.412	60966.	44.774	89334.
1750.00	53.593	36.119	89.711	63208.	44.892	93787.
1800.00	54.614	36.364	90.978	65455.	45.004	98305.
1850.00	55.613	36.599	92.212	67708.	45.111	102884.
1900.00	56.592	36.824	93.416	69966.	45.213	107525.
1950.00	57.552	37.041	94.592	72229.	45.311	112226.
2000.00	58.492	37.249	95.741	74497.	45.406	116984.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

THIS TABLE SUPERSEDES TABLE B-59 OF NBS REPORT 7437 AND TABLE B-37 OF NBS REPORT 6928.

TABLE B-60

THERMODYNAMIC FUNCTIONS FOR TUNGSTEN (W)
SOLID PHASE

GRAM MOLECULAR WT.=183.85 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.001	0.003	0.002	0.002
10.00	0.002	0.003	0.005	0.032	0.011	0.015
15.00	0.004	0.009	0.013	0.135	0.032	0.057
20.00	0.008	0.020	0.027	0.391	0.077	0.154
25.00	0.014	0.040	0.054	0.991	0.172	0.349
30.00	0.024	0.073	0.097	2.201	0.322	0.719
35.00	0.039	0.123	0.162	4.310	0.530	1.358
40.00	0.059	0.190	0.249	7.587	0.788	2.376
45.00	0.086	0.272	0.359	12.252	1.082	3.886
50.00	0.120	0.369	0.489	18.437	1.393	5.996
55.00	0.160	0.476	0.636	26.176	1.701	8.801
60.00	0.206	0.591	0.797	35.441	2.003	12.378
65.00	0.258	0.711	0.969	46.188	2.293	16.789
70.00	0.315	0.833	1.149	58.342	2.566	22.081
75.00	0.377	0.958	1.335	71.825	2.824	28.288
80.00	0.443	1.082	1.525	86.546	3.059	35.436
85.00	0.512	1.204	1.716	102.36	3.266	43.539
90.00	0.584	1.325	1.909	119.21	3.477	52.602
95.00	0.659	1.443	2.103	137.11	3.674	62.631
100.00	0.736	1.559	2.295	155.88	3.830	73.625
105.00	0.815	1.671	2.486	175.40	3.983	85.578
110.00	0.895	1.779	2.674	195.69	4.128	98.478
115.00	0.977	1.884	2.860	216.63	4.245	112.32
120.00	1.059	1.984	3.043	238.14	4.358	127.08
125.00	1.142	2.082	3.224	260.21	4.469	142.75
130.00	1.225	2.175	3.401	282.80	4.568	159.31
135.00	1.309	2.266	3.575	305.88	4.663	176.75
140.00	1.393	2.353	3.746	329.42	4.750	195.05
145.00	1.477	2.437	3.914	353.37	4.829	214.21
150.00	1.561	2.518	4.079	377.70	4.902	234.19
155.00	1.645	2.596	4.241	402.38	4.968	254.99
160.00	1.729	2.671	4.400	427.37	5.027	276.60
165.00	1.812	2.743	4.555	452.64	5.081	298.99
170.00	1.895	2.813	4.708	478.17	5.131	322.15
175.00	1.977	2.880	4.857	503.95	5.177	346.06
180.00	2.060	2.944	5.004	529.94	5.221	370.71
185.00	2.141	3.006	5.147	556.15	5.261	396.09
190.00	2.222	3.066	5.288	582.55	5.300	422.18
195.00	2.302	3.124	5.426	609.15	5.338	448.97
200.00	2.382	3.180	5.562	635.93	5.374	476.44
205.00	2.461	3.234	5.695	662.88	5.408	504.58
210.00	2.540	3.286	5.826	690.01	5.442	533.38
215.00	2.618	3.336	5.954	717.30	5.474	562.83
220.00	2.695	3.385	6.080	744.74	5.505	592.92
225.00	2.772	3.433	6.204	772.34	5.534	623.63
230.00	2.848	3.479	6.326	800.08	5.562	654.96
235.00	2.923	3.523	6.446	827.96	5.589	686.89
240.00	2.998	3.567	6.564	855.97	5.614	719.42
245.00	3.072	3.609	6.680	884.09	5.637	752.53
250.00	3.145	3.649	6.794	912.33	5.659	786.22
255.00	3.218	3.689	6.906	940.68	5.679	820.47
260.00	3.290	3.727	7.017	969.12	5.697	855.28
265.00	3.361	3.765	7.126	997.65	5.714	890.63
270.00	3.432	3.801	7.233	1026.3	5.731	926.53
273.15	3.476	3.823	7.299	1044.3	5.741	949.42
275.00	3.502	3.836	7.338	1055.0	5.746	962.96
280.00	3.571	3.870	7.442	1083.7	5.761	999.91
285.00	3.640	3.904	7.544	1112.6	5.776	1037.4
290.00	3.708	3.936	7.644	1141.5	5.790	1075.3
295.00	3.776	3.968	7.743	1170.5	5.802	1113.8
298.15	3.818	3.987	7.805	1188.7	5.810	1138.3
300.00	3.843	3.998	7.841	1199.5	5.814	1152.8

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-60(CONT.)

THERMODYNAMIC FUNCTIONS FOR TUNGSTEN (W)
SOLID PHASE

GRAM MOLECULAR WT.=183.85 GRAMS　　1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
300.00	3.843	3.998	7.841	1199.5	5.814	1152.8
310.00	3.975	4.057	8.032	1257.7	5.834	1232.1
320.00	4.104	4.113	8.217	1316.2	5.851	1313.4
330.00	4.232	4.166	8.398	1374.8	5.867	1396.5
340.00	4.357	4.216	8.573	1433.5	5.883	1481.3
350.00	4.480	4.264	8.744	1492.4	5.899	1567.9
360.00	4.601	4.310	8.910	1551.5	5.915	1656.2
370.00	4.719	4.353	9.072	1610.7	5.930	1746.1
373.15	4.756	4.367	9.123	1629.4	5.934	1774.8
380.00	4.836	4.395	9.231	1670.1	5.944	1837.6
390.00	4.951	4.435	9.385	1729.6	5.959	1930.7
400.00	5.063	4.473	9.536	1789.3	5.972	2025.3
425.00	5.337	4.562	9.900	1939.0	6.006	2268.3
450.00	5.600	4.643	10.244	2089.5	6.037	2520.1
475.00	5.853	4.718	10.571	2240.8	6.067	2780.4
500.00	6.097	4.786	10.883	2392.9	6.096	3048.6
550.00	6.559	4.907	11.466	2699.0	6.150	3607.5
600.00	6.991	5.013	12.004	3007.8	6.200	4194.4
650.00	7.396	5.106	12.502	3319.0	6.248	4807.2
700.00	7.777	5.189	12.967	3632.6	6.295	5444.0
750.00	8.138	5.265	13.403	3948.4	6.339	6103.7
800.00	8.480	5.333	13.813	4266.5	6.382	6784.2
850.00	8.805	5.396	14.201	4586.6	6.424	7484.6
900.00	9.116	5.454	14.570	4908.9	6.465	8204.0
950.00	9.412	5.509	14.920	5233.2	6.506	8941.3
1000.00	9.696	5.559	15.255	5559.4	6.545	9695.8
1050.00	9.968	5.607	15.575	5887.7	6.584	10467.
1100.00	10.230	5.653	15.883	6217.9	6.623	11253.
1150.00	10.482	5.696	16.178	6550.0	6.661	12055.
1200.00	10.726	5.737	16.462	6884.0	6.699	12871.
1250.00	10.961	5.776	16.736	7219.8	6.736	13701.
1300.00	11.188	5.814	17.001	7557.6	6.774	14544.
1350.00	11.408	5.850	17.258	7897.2	6.810	15401.
1400.00	11.621	5.885	17.506	8238.6	6.847	16270.
1450.00	11.828	5.919	17.747	8581.9	6.884	17151.
1500.00	12.030	5.951	17.981	8927.0	6.920	18044.
1550.00	12.225	5.983	18.208	9273.9	6.956	18949.
1600.00	12.416	6.014	18.430	9622.6	6.992	19865.
1650.00	12.601	6.044	18.646	9973.1	7.028	20792.
1700.00	12.782	6.074	18.856	10325.	7.064	21730.
1750.00	12.959	6.103	19.061	10679.	7.099	22678.
1800.00	13.131	6.131	19.262	11035.	7.135	23636.
1850.00	13.299	6.158	19.458	11393.	7.170	24604.
1900.00	13.464	6.185	19.649	11752.	7.205	25581.
1950.00	13.625	6.212	19.837	12113.	7.241	26568.
2000.00	13.782	6.238	20.021	12476.	7.276	27565.
2050.00	13.937	6.264	20.201	12841.	7.311	28571.
2100.00	14.088	6.289	20.377	13207.	7.346	29585.
2150.00	14.236	6.314	20.551	13576.	7.381	30608.
2200.00	14.382	6.339	20.721	13946.	7.416	31640.
2250.00	14.525	6.363	20.888	14317.	7.450	32680.
2300.00	14.665	6.387	21.052	14691.	7.485	33729.
2350.00	14.802	6.411	21.213	15066.	7.520	34785.
2400.00	14.937	6.434	21.372	15443.	7.555	35850.
2450.00	15.070	6.458	21.528	15821.	7.589	36922.
2500.00	15.201	6.481	21.682	16201.	7.624	38003.
2600.00	15.456	6.526	21.982	16967.	7.693	40186.
2700.00	15.703	6.570	22.274	17740.	7.762	42399.
2800.00	15.943	6.614	22.557	18520.	7.831	44640.
2900.00	16.176	6.657	22.833	19306.	7.899	46910.
3000.00	16.402	6.700	23.102	20100.	7.968	49207.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-61

THERMODYNAMIC FUNCTIONS FOR TUNGSTEN DIOXIDE ($W\ O_2$)
SOLID PHASE

GRAM MOLECULAR WT.=215.8488 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.000	0.001	0.001	0.001
10.00	0.001	0.002	0.003	0.021	0.010	0.007
15.00	0.003	0.010	0.013	0.154	0.047	0.042
20.00	0.008	0.026	0.034	0.516	0.103	0.154
25.00	0.016	0.050	0.066	1.257	0.201	0.398
30.00	0.028	0.087	0.115	2.602	0.344	0.843
35.00	0.045	0.136	0.181	4.776	0.533	1.576
40.00	0.067	0.200	0.267	8.002	0.763	2.690
45.00	0.095	0.277	0.372	12.465	1.027	4.281
50.00	0.129	0.366	0.495	18.322	1.319	6.442
55.00	0.168	0.467	0.635	25.676	1.623	9.261
60.00	0.214	0.576	0.790	34.555	1.931	12.818
65.00	0.264	0.693	0.957	45.014	2.254	17.178
70.00	0.320	0.816	1.136	57.106	2.583	22.405
75.00	0.381	0.945	1.325	70.844	2.912	28.554
80.00	0.446	1.078	1.524	86.232	3.244	35.674
85.00	0.515	1.215	1.730	103.28	3.573	43.806
90.00	0.589	1.355	1.944	121.96	3.903	52.989
95.00	0.666	1.498	2.164	142.31	4.235	63.256
100.00	0.746	1.643	2.389	164.31	4.565	74.637
105.00	0.830	1.790	2.620	187.95	4.891	87.159
110.00	0.917	1.938	2.855	213.21	5.211	100.84
115.00	1.006	2.087	3.094	240.06	5.528	115.72
120.00	1.098	2.237	3.336	268.49	5.842	131.79
125.00	1.193	2.388	3.580	298.47	6.153	149.08
130.00	1.289	2.539	3.828	330.01	6.460	167.60
135.00	1.388	2.689	4.077	363.07	6.763	187.36
140.00	1.488	2.840	4.329	397.63	7.060	208.37
145.00	1.591	2.991	4.581	433.66	7.352	230.65
150.00	1.695	3.141	4.835	471.13	7.637	254.19
155.00	1.800	3.290	5.090	510.01	7.914	279.00
160.00	1.907	3.439	5.346	550.26	8.185	305.09
165.00	2.015	3.587	5.602	591.84	8.447	332.46
170.00	2.124	3.734	5.858	634.72	8.702	361.11
175.00	2.235	3.879	6.114	678.85	8.949	391.04
180.00	2.346	4.023	6.369	724.20	9.190	422.25
185.00	2.458	4.166	6.624	770.74	9.424	454.73
190.00	2.571	4.308	6.879	818.43	9.652	488.49
195.00	2.685	4.447	7.132	867.25	9.874	523.51
200.00	2.799	4.586	7.385	917.16	10.091	559.81
205.00	2.914	4.723	7.637	968.15	10.304	597.36
210.00	3.029	4.858	7.887	1020.2	10.511	636.17
215.00	3.145	4.992	8.137	1073.3	10.714	676.23
220.00	3.262	5.124	8.386	1127.3	10.911	717.54
225.00	3.378	5.255	8.633	1182.4	11.102	760.09
230.00	3.495	5.384	8.879	1238.3	11.287	803.87
235.00	3.612	5.512	9.124	1295.2	11.466	848.88
240.00	3.730	5.637	9.367	1353.0	11.638	895.11
245.00	3.847	5.762	9.609	1411.6	11.805	942.55
250.00	3.965	5.884	9.849	1471.0	11.967	991.19
255.00	4.082	6.005	10.087	1531.3	12.124	1041.0
260.00	4.200	6.124	10.324	1592.3	12.277	1092.1
265.00	4.318	6.242	10.560	1654.0	12.425	1144.3
270.00	4.436	6.357	10.793	1716.5	12.570	1197.7
273.15	4.510	6.430	10.939	1756.2	12.659	1231.9
275.00	4.553	6.472	11.025	1779.7	12.711	1252.2
280.00	4.671	6.584	11.255	1843.6	12.850	1307.9
285.00	4.789	6.695	11.484	1908.2	12.987	1364.8
290.00	4.906	6.805	11.711	1973.5	13.122	1422.7
295.00	5.023	6.913	11.937	2039.4	13.257	1481.9
298.15	5.097	6.981	12.078	2081.3	13.342	1519.7
300.00	5.140	7.020	12.160	2106.0	13.391	1542.1

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-61(CONT.)

THERMODYNAMIC FUNCTIONS FOR TUNGSTEN DIOXIDE (WO_2)
SOLID PHASE

GRAM MOLECULAR WT.=215.8488 GRAMS 1 CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
300.00	5.140	7.020	12.160	2106.0	13.391	1542.1
310.00	5.374	7.230	12.604	2241.3	13.650	1665.9
320.00	5.607	7.434	13.041	2379.0	13.889	1794.2
330.00	5.839	7.633	13.472	2519.0	14.102	1926.7
340.00	6.069	7.826	13.896	2660.9	14.291	2063.6
350.00	6.299	8.013	14.312	2804.7	14.462	2204.6
360.00	6.527	8.195	14.722	2950.1	14.620	2349.8
370.00	6.754	8.370	15.125	3097.1	14.769	2499.0
373.15	6.825	8.425	15.250	3143.7	14.815	2546.9
380.00	6.980	8.541	15.520	3245.5	14.911	2652.3
390.00	7.204	8.706	15.909	3395.3	15.045	2809.4
400.00	7.426	8.866	16.292	3546.4	15.172	2970.4
425.00	7.975	9.246	17.221	3929.4	15.461	3389.4
450.00	8.514	9.598	18.112	4319.2	15.718	3831.1
475.00	9.042	9.926	18.968	4715.1	15.949	4294.7
500.00	9.559	10.233	19.791	5116.5	16.160	4779.3
550.00	10.560	10.789	21.350	5934.0	16.533	5808.3
600.00	11.521	11.282	22.802	6769.0	16.860	6912.5
650.00	12.442	11.722	24.164	7619.5	17.154	8087.0
700.00	13.325	12.120	25.445	8484.0	17.425	9327.5
750.00	14.174	12.482	26.656	9361.6	17.677	10630.
800.00	14.990	12.814	27.804	10251.	17.916	11992.
850.00	15.776	13.121	28.898	11153.	18.145	13410.
900.00	16.534	13.407	29.941	12066.	18.366	14881.
950.00	17.266	13.673	30.940	12990.	18.581	16403.
1000.00	17.974	13.924	31.898	13924.	18.790	17974.
1050.00	18.659	14.161	32.820	14869.	18.995	19592.
1100.00	19.323	14.385	33.708	15823.	19.197	21256.
1150.00	19.968	14.598	34.566	16788.	19.395	22963.
1200.00	20.593	14.802	35.396	17763.	19.592	24712.
1250.00	21.201	14.998	36.199	18747.	19.786	26502.
1300.00	21.793	15.186	36.979	19741.	19.978	28331.
1350.00	22.370	15.367	37.737	20745.	20.169	30199.
1400.00	22.932	15.542	38.474	21758.	20.359	32105.
1450.00	23.480	15.711	39.191	22781.	20.548	34046.
1500.00	24.016	15.875	39.891	23813.	20.736	36023.
1550.00	24.539	16.035	40.574	24855.	20.922	38035.
1600.00	25.050	16.191	41.241	25905.	21.109	40081.
1650.00	25.551	16.343	41.894	26965.	21.294	42159.
1700.00	26.041	16.491	42.532	28035.	21.479	44270.
1750.00	26.521	16.636	43.157	29113.	21.664	46412.
1800.00	26.992	16.778	43.770	30201.	21.848	48585.
1850.00	27.453	16.918	44.371	31298.	22.031	50789.
1900.00	27.906	17.055	44.961	32404.	22.214	53022.
1950.00	28.351	17.189	45.541	33519.	22.397	55285.
2000.00	28.788	17.322	46.110	34644.	22.580	57576.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-62

THERMODYNAMIC FUNCTIONS FOR TUNGSTEN TRIOXIDE (WO_3)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=231.8482 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
SOLID PHASE (ALPHA)						
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.001	0.003	0.002	0.002
10.00	0.002	0.006	0.008	0.059	0.030	0.020
15.00	0.008	0.029	0.037	0.437	0.132	0.120
20.00	0.022	0.073	0.095	1.462	0.291	0.439
25.00	0.045	0.141	0.186	3.518	0.549	1.125
30.00	0.079	0.236	0.315	7.084	0.888	2.361
35.00	0.124	0.357	0.481	12.483	1.278	4.335
40.00	0.180	0.498	0.678	19.901	1.690	7.219
45.00	0.248	0.653	0.901	29.400	2.114	11.157
50.00	0.325	0.823	1.148	41.144	2.598	16.271
55.00	0.412	1.008	1.420	55.430	3.107	22.683
60.00	0.508	1.202	1.710	72.119	3.567	30.503
65.00	0.612	1.402	2.015	91.134	4.040	39.810
70.00	0.724	1.607	2.331	112.51	4.511	50.669
75.00	0.842	1.816	2.658	136.24	4.978	63.139
80.00	0.966	2.029	2.995	162.30	5.449	77.268
85.00	1.095	2.244	3.339	190.70	5.906	93.099
90.00	1.230	2.460	3.689	221.35	6.358	110.67
95.00	1.368	2.677	4.045	254.29	6.817	130.00
100.00	1.511	2.895	4.406	289.52	7.274	151.13
105.00	1.658	3.114	4.772	327.00	7.716	174.07
110.00	1.808	3.333	5.141	366.63	8.131	198.85
115.00	1.961	3.550	5.511	408.29	8.533	225.48
120.00	2.116	3.766	5.883	451.95	8.928	253.97
125.00	2.274	3.981	6.255	497.59	9.325	284.31
130.00	2.435	4.194	6.628	545.17	9.708	316.52
135.00	2.597	4.405	7.002	594.65	10.083	350.59
140.00	2.761	4.614	7.375	645.98	10.445	386.54
145.00	2.927	4.821	7.748	699.08	10.793	424.34
150.00	3.093	5.026	8.119	753.89	11.130	464.01
155.00	3.262	5.228	8.490	810.35	11.453	505.54
160.00	3.431	5.428	8.858	868.40	11.764	548.91
165.00	3.601	5.624	9.225	927.98	12.065	594.11
170.00	3.771	5.818	9.589	989.03	12.354	641.15
175.00	3.943	6.009	9.951	1051.5	12.633	690.00
180.00	4.115	6.196	10.311	1115.3	12.902	740.66
185.00	4.287	6.381	10.668	1180.5	13.165	793.11
190.00	4.460	6.563	11.023	1247.0	13.422	847.34
195.00	4.632	6.742	11.375	1314.7	13.676	903.33
200.00	4.805	6.919	11.724	1383.7	13.928	961.08
205.00	4.978	7.093	12.071	1454.0	14.178	1020.6
210.00	5.151	7.264	12.416	1525.5	14.423	1081.8
215.00	5.324	7.434	12.758	1598.2	14.662	1144.7
220.00	5.497	7.601	13.098	1672.1	14.892	1209.4
225.00	5.670	7.765	13.435	1747.1	15.111	1275.7
230.00	5.842	7.927	13.769	1823.2	15.318	1343.7
235.00	6.014	8.086	14.101	1900.3	15.515	1413.4
240.00	6.186	8.243	14.429	1978.3	15.704	1484.7
245.00	6.358	8.397	14.755	2057.3	15.886	1557.7
250.00	6.529	8.549	15.078	2137.2	16.064	1632.3
255.00	6.700	8.698	15.398	2218.0	16.239	1708.4
260.00	6.870	8.845	15.715	2299.6	16.411	1786.2
265.00	7.040	8.989	16.029	2382.1	16.581	1865.6
270.00	7.209	9.131	16.340	2465.4	16.748	1946.5
273.15	7.316	9.220	16.535	2518.3	16.851	1998.3
275.00	7.378	9.271	16.649	2549.5	16.911	2029.0
280.00	7.546	9.409	16.955	2634.5	17.068	2113.0
285.00	7.714	9.545	17.259	2720.2	17.219	2198.5
290.00	7.881	9.678	17.559	2806.7	17.361	2285.6
295.00	8.048	9.809	17.857	2893.8	17.493	2374.1
298.15	8.152	9.891	18.044	2949.0	17.571	2430.7
300.00	8.214	9.939	18.152	2981.6	17.615	2464.1

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-62(CONT.)

THERMODYNAMIC FUNCTIONS FOR TUNGSTEN TRIOXIDE ($W O_3$)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=231.8482 GRAMS 1 CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T	$-(G_T^0-H_0^0)/T$	$(H_T^0-H_0^0)/T$	$(S_T^0-S_0^0)$	$(H_T^0-H_0^0)$	C_P^0	$-(G_T^0-H_0^0)$
DEG K	CAL/DEG MOLE	CAL/DEG MOLE	CAL/DEG MOLE	CAL/MOLE	CAL/DEG MOLE	CAL/MOLE
			SOLID PHASE (ALPHA)			
300.00	8.214	9.939	18.152	2981.6	17.615	2464.1
310.00	8.544	10.190	18.734	3158.9	17.840	2648.6
320.00	8.871	10.432	19.304	3338.4	18.062	2838.8
330.00	9.196	10.667	19.863	3520.2	18.303	3034.6
340.00	9.518	10.896	20.413	3704.5	18.561	3236.0
350.00	9.837	11.118	20.955	3891.4	18.820	3442.9
360.00	10.153	11.336	21.489	4080.8	19.062	3655.1
370.00	10.467	11.547	22.014	4272.6	19.284	3872.6
373.15	10.565	11.613	22.178	4333.4	19.349	3942.2
380.00	10.777	11.754	22.531	4466.4	19.486	4095.3
390.00	11.085	11.954	23.040	4662.2	19.673	4323.2
400.00	11.390	12.150	23.540	4859.9	19.850	4556.1
425.00	12.141	12.615	24.756	5361.2	20.249	5159.9
450.00	12.874	13.049	25.923	5871.9	20.598	5793.5
475.00	13.591	13.454	27.045	6390.8	20.906	6455.7
500.00	14.291	13.834	28.125	6916.9	21.182	7145.4
550.00	15.642	14.524	30.166	7988.3	21.658	8603.3
600.00	16.933	15.136	32.069	9081.5	22.060	10160.
650.00	18.166	15.682	33.848	10193.	22.411	11808.
700.00	19.347	16.174	35.521	11322.	22.724	13543.
750.00	20.478	16.621	37.099	12465.	23.009	15359.
800.00	21.564	17.028	38.592	13623.	23.273	17251.
850.00	22.608	17.403	40.011	14792.	23.521	19217.
900.00	23.612	17.749	41.362	15974.	23.756	21251.
950.00	24.581	18.072	42.652	17168.	23.981	23352.
1000.00	25.515	18.372	43.888	18372.	24.198	25515.
1050.00	26.419	18.655	45.074	19588.	24.408	27740.
			SOLID PHASE (BETA)			
1050.00	26.419	19.046	45.465	19999.	23.709	27740.
1100.00	27.310	19.261	46.571	21188.	23.848	30041.
1150.00	28.170	19.464	47.634	22383.	23.987	32396.
1200.00	29.003	19.655	48.658	23586.	24.126	34804.
1250.00	29.809	19.837	49.646	24796.	24.265	37261.
1300.00	30.590	20.010	50.600	26013.	24.404	39768.
1350.00	31.349	20.175	51.524	27236.	24.543	42321.
1400.00	32.085	20.334	52.419	28467.	24.682	44919.
1450.00	32.802	20.486	53.287	29705.	24.821	47562.
1500.00	33.499	20.633	54.131	30949.	24.960	50248.
1550.00	34.177	20.775	54.952	32201.	25.099	52975.
1600.00	34.839	20.912	55.751	33459.	25.238	55743.
1650.00	35.485	21.045	56.530	34724.	25.377	58550.
1700.00	36.115	21.175	57.289	35997.	25.516	61395.
1745.00	36.670	21.288	57.958	37148.	25.641	63988.
			LIQUID PHASE			
1745.00	36.670	31.335	68.004	54679.	31.500	63988.
1750.00	36.759	31.335	68.094	54836.	31.500	64329.
1800.00	37.642	31.340	68.982	56411.	31.500	67756.
1850.00	38.501	31.344	69.845	57986.	31.500	71226.
1900.00	39.337	31.348	70.685	59561.	31.500	74740.
1950.00	40.151	31.352	71.503	61136.	31.500	78294.
2000.00	40.945	31.356	72.300	62711.	31.500	81890.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-63

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM MONOTUNGSTATE (MG W O_4)
SOLID PHASE

GRAM MOLECULAR WT.=272.1596 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.001	0.003	0.002	0.002
10.00	0.002	0.006	0.008	0.059	0.030	0.020
15.00	0.008	0.029	0.037	0.437	0.132	0.120
20.00	0.022	0.073	0.095	1.462	0.291	0.439
25.00	0.045	0.141	0.186	3.523	0.551	1.125
30.00	0.079	0.238	0.316	7.129	0.904	2.364
35.00	0.124	0.362	0.487	12.684	1.329	4.356
40.00	0.182	0.513	0.695	20.510	1.810	7.296
45.00	0.253	0.686	0.938	30.852	2.333	11.366
50.00	0.335	0.878	1.212	43.890	2.886	16.730
55.00	0.428	1.086	1.513	59.707	3.438	23.535
60.00	0.532	1.305	1.836	78.282	3.998	31.901
65.00	0.645	1.535	2.180	99.757	4.597	41.933
70.00	0.768	1.775	2.543	124.28	5.217	53.732
75.00	0.899	2.026	2.925	151.95	5.851	67.394
80.00	1.038	2.285	3.323	182.81	6.495	83.005
85.00	1.184	2.552	3.736	216.92	7.150	100.65
90.00	1.338	2.826	4.163	254.32	7.813	120.39
95.00	1.498	3.106	4.604	295.05	8.478	142.30
100.00	1.664	3.391	5.055	339.09	9.135	166.45
105.00	1.837	3.680	5.517	386.39	9.784	192.87
110.00	2.015	3.972	5.987	436.91	10.422	221.63
115.00	2.198	4.266	6.464	490.59	11.051	252.75
120.00	2.386	4.562	6.947	547.41	11.673	286.28
125.00	2.578	4.859	7.436	607.33	12.293	322.23
130.00	2.774	5.156	7.931	670.32	12.901	360.65
135.00	2.974	5.454	8.429	736.32	13.498	401.54
140.00	3.178	5.752	8.930	805.27	14.081	444.94
145.00	3.385	6.049	9.434	877.10	14.648	490.85
150.00	3.595	6.345	9.940	951.72	15.199	539.28
155.00	3.808	6.639	10.447	1029.1	15.733	590.25
160.00	4.023	6.931	10.955	1109.0	16.251	643.76
165.00	4.241	7.221	11.463	1191.5	16.753	699.80
170.00	4.461	7.509	11.970	1276.5	17.240	758.38
175.00	4.683	7.794	12.477	1363.9	17.713	819.50
180.00	4.906	8.076	12.982	1453.6	18.173	883.15
185.00	5.131	8.355	13.486	1545.6	18.619	949.32
190.00	5.358	8.631	13.989	1639.8	19.054	1018.0
195.00	5.586	8.903	14.489	1736.1	19.478	1089.2
200.00	5.814	9.173	14.987	1834.6	19.890	1162.9
205.00	6.044	9.439	15.483	1935.0	20.293	1239.1
210.00	6.275	9.702	15.977	2037.5	20.685	1317.7
215.00	6.506	9.962	16.468	2141.9	21.067	1398.8
220.00	6.738	10.219	16.957	2248.1	21.437	1482.4
225.00	6.971	10.472	17.443	2356.2	21.795	1568.4
230.00	7.204	10.722	17.926	2466.1	22.143	1656.8
235.00	7.437	10.969	18.405	2577.6	22.479	1747.7
240.00	7.670	11.212	18.882	2690.8	22.805	1840.9
245.00	7.904	11.452	19.356	2805.7	23.122	1936.5
250.00	8.138	11.688	19.826	2922.0	23.430	2034.4
255.00	8.371	11.921	20.293	3039.9	23.730	2134.7
260.00	8.605	12.151	20.756	3159.3	24.021	2237.3
265.00	8.839	12.378	21.217	3280.1	24.305	2342.3
270.00	9.072	12.601	21.674	3402.4	24.581	2449.5
273.15	9.219	12.740	21.960	3480.1	24.751	2518.2
275.00	9.306	12.822	22.127	3525.9	24.851	2559.0
280.00	9.538	13.039	22.577	3650.9	25.115	2670.8
285.00	9.771	13.253	23.024	3777.1	25.377	2784.8
290.00	10.003	13.464	23.468	3904.6	25.639	2901.0
295.00	10.235	13.673	23.908	4033.5	25.902	3019.5
298.15	10.381	13.803	24.184	4115.3	26.070	3095.2
300.00	10.467	13.879	24.346	4163.7	26.170	3140.1

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-64

THERMODYNAMIC FUNCTIONS FOR LITHIUM METATITANATE $(LI_2TI\ O_3)$
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=109.7762 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
SOLID PHASE (ALPHA)						
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.001	0.002	0.001	0.001
10.00	0.001	0.003	0.004	0.028	0.014	0.009
15.00	0.004	0.014	0.018	0.207	0.063	0.057
20.00	0.010	0.035	0.045	0.694	0.139	0.207
25.00	0.021	0.068	0.089	1.688	0.269	0.534
30.00	0.038	0.116	0.154	3.480	0.457	1.131
35.00	0.060	0.181	0.242	6.344	0.698	2.110
40.00	0.090	0.263	0.353	10.536	0.986	3.586
45.00	0.126	0.362	0.488	16.276	1.316	5.679
50.00	0.170	0.475	0.645	23.757	1.681	8.503
55.00	0.221	0.603	0.824	33.140	2.078	12.166
60.00	0.280	0.744	1.023	44.619	2.523	16.775
65.00	0.345	0.900	1.245	58.470	3.025	22.435
70.00	0.418	1.070	1.488	74.930	3.564	29.259
75.00	0.498	1.256	1.754	94.177	4.143	37.356
80.00	0.585	1.456	2.041	116.44	4.768	46.833
85.00	0.680	1.669	2.349	141.88	5.410	57.800
90.00	0.782	1.895	2.677	170.57	6.066	70.358
95.00	0.891	2.132	3.023	202.58	6.744	84.600
100.00	1.006	2.380	3.386	238.03	7.439	100.62
105.00	1.128	2.638	3.766	276.98	8.139	118.49
110.00	1.257	2.904	4.161	319.42	8.838	138.30
115.00	1.392	3.177	4.569	365.36	9.539	160.13
120.00	1.533	3.457	4.990	414.82	10.247	184.02
125.00	1.680	3.742	5.423	467.80	10.944	210.05
130.00	1.833	4.033	5.866	524.26	11.636	238.27
135.00	1.991	4.327	6.318	584.15	12.319	268.72
140.00	2.153	4.624	6.778	647.43	12.989	301.45
145.00	2.321	4.924	7.245	714.02	13.647	336.51
150.00	2.493	5.226	7.719	783.87	14.289	373.91
155.00	2.669	5.528	8.197	856.89	14.916	413.70
160.00	2.849	5.831	8.681	933.00	15.527	455.90
165.00	3.033	6.134	9.168	1012.1	16.120	500.51
170.00	3.221	6.436	9.657	1094.2	16.696	547.58
175.00	3.412	6.737	10.149	1179.1	17.253	597.09
180.00	3.606	7.037	10.643	1266.7	17.793	649.07
185.00	3.803	7.335	11.138	1357.0	18.316	703.52
190.00	4.002	7.631	11.633	1449.8	18.822	760.45
195.00	4.204	7.924	12.128	1545.2	19.314	819.85
200.00	4.409	8.215	12.623	1642.9	19.792	881.73
205.00	4.615	8.503	13.118	1743.1	20.256	946.09
210.00	4.823	8.788	13.611	1845.5	20.706	1012.9
215.00	5.033	9.070	14.104	1950.1	21.140	1082.2
220.00	5.245	9.349	14.594	2056.8	21.560	1153.9
225.00	5.458	9.625	15.084	2165.7	21.965	1228.1
230.00	5.673	9.898	15.571	2276.5	22.356	1304.8
235.00	5.889	10.167	16.056	2389.2	22.734	1383.8
240.00	6.106	10.432	16.538	2503.8	23.100	1465.3
245.00	6.323	10.695	17.018	2620.2	23.453	1549.2
250.00	6.542	10.953	17.495	2738.3	23.795	1635.5
255.00	6.761	11.208	17.970	2858.1	24.125	1724.2
260.00	6.982	11.460	18.441	2979.5	24.442	1815.2
265.00	7.202	11.708	18.910	3102.5	24.746	1908.6
270.00	7.423	11.952	19.375	3227.0	25.039	2004.3
273.15	7.563	12.104	19.667	3306.1	25.218	2065.8
275.00	7.645	12.192	19.837	3352.9	25.322	2102.3
280.00	7.867	12.429	20.296	3480.2	25.597	2202.7
285.00	8.089	12.663	20.751	3608.8	25.865	2305.3
290.00	8.311	12.893	21.203	3738.8	26.130	2410.2
295.00	8.533	13.119	21.652	3870.1	26.391	2517.3
298.15	8.673	13.260	21.933	3953.5	26.554	2585.9
300.00	8.756	13.342	22.098	4002.7	26.650	2626.7

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-64(CONT.)

THERMODYNAMIC FUNCTIONS FOR LITHIUM METATITANATE ($LI_2TI\ O_3$)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=109.7762 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T	$-(G^0_T-H^0_0)/T$	$(H^0_T-H^0_0)/T$	$(S^0_T-S^0_0)$	$(H^0_T-H^0_0)$	C^0_P	$-(G^0_T-H^0_0)$
DEG K	CAL/DEG MOLE	CAL/DEG MOLE	CAL/DEG MOLE	CAL/MOLE	CAL/DEG MOLE	CAL/MOLE
			SOLID PHASE (ALPHA)			
300.00	8.756	13.342	22.098	4002.7	26.650	2626.7
310.00	9.200	13.780	22.980	4271.8	27.158	2852.1
320.00	9.644	14.206	23.850	4545.8	27.645	3086.2
330.00	10.088	14.620	24.708	4824.6	28.101	3329.0
340.00	10.530	15.023	25.553	5107.7	28.521	3580.4
350.00	10.972	15.414	26.386	5394.9	28.905	3840.1
360.00	11.411	15.794	27.205	5685.7	29.259	4108.0
370.00	11.849	16.162	28.011	5980.0	29.587	4384.1
373.15	11.986	16.276	28.262	6073.3	29.686	4472.7
380.00	12.285	16.519	28.804	6277.4	29.892	4668.2
390.00	12.718	16.866	29.584	6577.8	30.178	4960.2
400.00	13.150	17.202	30.352	6880.9	30.445	5259.8
425.00	14.217	17.999	32.216	7649.7	31.046	6042.1
450.00	15.267	18.739	34.006	8432.5	31.567	6870.0
475.00	16.299	19.426	35.725	9227.5	32.023	7741.8
500.00	17.311	20.067	37.378	10033.	32.427	8655.7
550.00	19.279	21.223	40.502	11672.	33.118	10604.
600.00	21.170	22.239	43.409	13343.	33.693	12702.
650.00	22.987	23.139	46.126	15040.	34.186	14941.
700.00	24.732	23.944	48.675	16761.	34.619	17312.
750.00	26.408	24.669	51.077	18502.	35.009	19806.
800.00	28.021	25.327	53.348	20261.	35.365	22417.
850.00	29.575	25.927	55.502	22038.	35.696	25139.
900.00	31.073	26.478	57.551	23831.	36.006	27965.
950.00	32.518	26.988	59.506	25638.	36.301	30892.
1000.00	33.915	27.460	61.375	27460.	36.582	33915.
1050.00	35.265	27.901	63.167	29296.	36.853	37028.
1100.00	36.573	28.314	64.887	31146.	37.115	40230.
1150.00	37.840	28.702	66.542	33008.	37.370	43516.
1200.00	39.069	29.069	68.138	34883.	37.619	46883.
1250.00	40.263	29.416	69.679	36770.	37.863	50329.
1300.00	41.423	29.745	71.169	38669.	38.103	53850.
1350.00	42.552	30.059	72.611	40580.	38.339	57445.
1400.00	43.651	30.359	74.010	42503.	38.572	61111.
1450.00	44.721	30.646	75.367	44437.	38.802	64845.
1485.00	45.454	30.840	76.294	45798.	38.962	67499.
			SOLID PHASE (BETA)			
1485.00	45.454	32.692	78.146	48548.	42.080	67499.
1500.00	45.783	32.787	78.570	49180.	42.200	68675.
1550.00	46.863	33.097	79.960	51300.	42.600	72638.
1600.00	47.919	33.400	81.319	53440.	43.000	76670.
1650.00	48.951	33.697	82.648	55600.	43.400	80770.
1700.00	49.962	33.988	83.950	57780.	43.800	84935.
1750.00	50.951	34.274	85.225	59980.	44.200	89164.
1800.00	51.920	34.556	86.476	62200.	44.600	93457.
1820.00	52.303	34.667	86.970	63094.	44.760	95191.
			LIQUID PHASE			
1820.00	52.303	49.134	101.44	89424.	48.000	95191.
1850.00	53.106	49.115	102.22	90864.	48.000	98246.
1900.00	54.415	49.086	103.50	93264.	48.000	103389.
1950.00	55.690	49.058	104.75	95664.	48.000	108596.
2000.00	56.932	49.032	105.96	98064.	48.000	113864.

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-65

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM METASILICATE (MG SI O_3)
SOLID PHASE

T DEG K = 273.15 + T DEG C

GRAM MOLECULAR WT.=100.3962 GRAMS

1 CAL=4.1840 ABS J

T DEG K	$-(G^0_T-H^0_0)/T$ $\frac{\text{CAL}}{\text{DEG MOLE}}$	$(H^0_T-H^0_0)/T$ $\frac{\text{CAL}}{\text{DEG MOLE}}$	$(S^0_T-S^0_0)$ $\frac{\text{CAL}}{\text{DEG MOLE}}$	$(H^0_T-H^0_0)$ $\frac{\text{CAL}}{\text{MOLE}}$	C^0_P $\frac{\text{CAL}}{\text{DEG MOLE}}$	$-(G^0_T-H^0_0)$ $\frac{\text{CAL}}{\text{MOLE}}$
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.000	0.001	0.001	0.001
10.00	0.001	0.002	0.003	0.020	0.010	0.007
15.00	0.003	0.010	0.013	0.150	0.045	0.041
20.00	0.008	0.025	0.033	0.502	0.101	0.150
25.00	0.015	0.049	0.064	1.224	0.196	0.387
30.00	0.027	0.084	0.112	2.533	0.336	0.820
35.00	0.044	0.133	0.177	4.656	0.521	1.534
40.00	0.066	0.195	0.261	7.820	0.752	2.621
45.00	0.093	0.272	0.365	12.243	1.024	4.177
50.00	0.126	0.362	0.488	18.120	1.332	6.303
55.00	0.165	0.465	0.631	25.585	1.657	9.093
60.00	0.211	0.579	0.790	34.753	2.020	12.636
65.00	0.262	0.706	0.968	45.869	2.433	17.022
70.00	0.319	0.844	1.164	59.114	2.868	22.343
75.00	0.382	0.994	1.377	74.576	3.320	28.687
80.00	0.452	1.154	1.606	92.336	3.785	36.137
85.00	0.527	1.323	1.849	112.44	4.257	44.770
90.00	0.607	1.499	2.106	134.93	4.742	54.655
95.00	0.693	1.683	2.376	159.86	5.232	65.856
100.00	0.784	1.872	2.657	187.22	5.712	78.433
105.00	0.880	2.066	2.947	216.98	6.193	92.438
110.00	0.981	2.265	3.246	249.17	6.686	107.92
115.00	1.086	2.468	3.554	283.84	7.181	124.91
120.00	1.196	2.675	3.870	320.96	7.665	143.47
125.00	1.309	2.884	4.193	360.48	8.142	163.63
130.00	1.426	3.095	4.521	402.37	8.612	185.41
135.00	1.547	3.308	4.855	446.59	9.073	208.85
140.00	1.671	3.522	5.193	493.09	9.526	233.97
145.00	1.799	3.737	5.535	541.83	9.970	260.79
150.00	1.929	3.952	5.881	592.77	10.405	289.33
155.00	2.062	4.167	6.229	645.87	10.831	319.60
160.00	2.198	4.382	6.579	701.07	11.247	351.62
165.00	2.336	4.596	6.932	758.32	11.653	385.40
170.00	2.476	4.809	7.285	817.58	12.050	420.94
175.00	2.619	5.022	7.640	878.81	12.438	458.25
180.00	2.763	5.233	7.996	941.95	12.817	497.35
185.00	2.909	5.443	8.352	1007.0	13.189	538.22
190.00	3.057	5.652	8.709	1073.8	13.552	580.87
195.00	3.207	5.859	9.066	1142.5	13.907	625.31
200.00	3.358	6.064	9.422	1212.9	14.254	671.52
205.00	3.510	6.268	9.778	1285.0	14.592	719.52
210.00	3.663	6.470	10.134	1358.8	14.922	769.31
215.00	3.818	6.671	10.489	1434.2	15.244	820.86
220.00	3.974	6.869	10.843	1511.2	15.558	874.19
225.00	4.130	7.066	11.196	1589.8	15.864	929.29
230.00	4.288	7.260	11.548	1669.8	16.162	986.15
235.00	4.446	7.453	11.898	1751.4	16.452	1044.8
240.00	4.605	7.643	12.248	1834.3	16.736	1105.1
245.00	4.764	7.832	12.596	1918.7	17.013	1167.2
250.00	4.924	8.018	12.942	2004.5	17.286	1231.1
255.00	5.085	8.202	13.287	2091.6	17.557	1296.7
260.00	5.246	8.385	13.631	2180.0	17.826	1364.0
265.00	5.407	8.565	13.973	2269.8	18.093	1433.0
270.00	5.569	8.744	14.313	2361.0	18.353	1503.7
273.15	5.671	8.856	14.527	2419.0	18.512	1549.1
275.00	5.731	8.921	14.653	2453.3	18.602	1576.1
280.00	5.894	9.096	14.990	2546.9	18.831	1650.2
285.00	6.056	9.269	15.325	2641.6	19.037	1726.0
290.00	6.219	9.439	15.658	2737.3	19.214	1803.4
295.00	6.382	9.606	15.987	2833.7	19.366	1882.6
298.15	6.484	9.709	16.194	2894.9	19.450	1933.2
300.00	6.544	9.770	16.314	2930.9	19.496	1963.3

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-65(CONT.)

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM METASILICATE (MG SI O_3)
SOLID PHASE

T DEG K = 273.15 + T DEG C
GRAM MOLECULAR WT.=100.3962 GRAMS 1 CAL=4.1840 ABS J

T DEG K	$-(G_T^0-H_0^0)/T$ CAL / DEG MOLE	$(H_T^0-H_0^0)/T$ CAL / DEG MOLE	$(S_T^0-S_0^0)$ CAL / DEG MOLE	$(H_T^0-H_0^0)$ CAL / MOLE	C_P^0 CAL / DEG MOLE	$-(G_T^0-H_0^0)$ CAL / MOLE
300.00	6.544	9.770	16.314	2930.9	19.496	1963.3
310.00	6.870	10.087	16.957	3127.0	19.731	2129.7
320.00	7.195	10.392	17.587	3325.6	19.990	2302.4
330.00	7.519	10.688	18.207	3527.0	20.312	2481.4
340.00	7.843	10.976	18.819	3732.0	20.680	2666.5
350.00	8.165	11.259	19.424	3940.7	21.054	2857.8
360.00	8.486	11.536	20.022	4153.0	21.404	3055.0
370.00	8.806	11.807	20.613	4368.6	21.720	3258.2
373.15	8.906	11.891	20.797	4437.2	21.813	3323.4
380.00	9.124	12.072	21.196	4587.3	22.007	3467.2
390.00	9.441	12.330	21.771	4808.7	22.272	3682.1
400.00	9.757	12.582	22.338	5032.7	22.521	3902.6
425.00	10.538	13.183	23.721	5602.9	23.087	4478.5
450.00	11.307	13.748	25.055	6186.4	23.582	5088.3
475.00	12.065	14.277	26.342	6781.5	24.018	5730.8
500.00	12.810	14.774	27.584	7386.9	24.408	6405.0
550.00	14.261	15.681	29.943	8624.6	25.080	7843.8
600.00	15.661	16.489	32.150	9893.2	25.649	9396.7
650.00	17.010	17.213	34.223	11188.	26.144	11057.
700.00	18.310	17.867	36.177	12507.	26.586	12817.
750.00	19.563	18.462	38.025	13847.	26.989	14672.
800.00	20.772	19.007	39.779	15205.	27.361	16618.
850.00	21.940	19.508	41.448	16582.	27.710	18649.
900.00	23.068	19.973	43.042	17976.	28.041	20761.
950.00	24.160	20.406	44.566	19386.	28.357	22952.
1000.00	25.217	20.812	46.029	20812.	28.662	25217.
1050.00	26.242	21.192	47.434	22252.	28.957	27554.
1100.00	27.236	21.552	48.788	23707.	29.245	29960.
1150.00	28.202	21.893	50.094	25176.	29.526	32432.
1200.00	29.140	22.216	51.357	26660.	29.802	34968.
1250.00	30.053	22.525	52.579	28157.	30.073	37567.
1300.00	30.943	22.821	53.763	29667.	30.340	40225.
1350.00	31.809	23.104	54.913	31191.	30.604	42943.
1400.00	32.654	23.377	56.031	32727.	30.866	45716.
1450.00	33.479	23.639	57.119	34277.	31.124	48545.
1500.00	34.285	23.893	58.178	35840.	31.381	51428.
1550.00	35.073	24.139	59.211	37415.	31.636	54363.
1600.00	35.843	24.377	60.220	39003.	31.889	57348.
1650.00	36.596	24.608	61.205	40604.	32.140	60384.
1700.00	37.334	24.834	62.168	42217.	32.391	63468.
1750.00	38.057	25.053	63.111	43843.	32.640	66601.
1800.00	38.766	25.267	64.034	45481.	32.888	69779.
1850.00	39.461	25.477	64.938	47132.	33.135	73004.
1900.00	40.144	25.681	65.825	48795.	33.382	76273.
1950.00	40.813	25.882	66.695	50470.	33.628	79586.
2000.00	41.471	26.079	67.550	52158.	33.873	82942.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-66

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM ORTHOSILICATE ($MG_2SI\ O_4$)
SOLID PHASE

GRAM MOLECULAR WT.=140.7076 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.000	0.001	0.001	0.001
10.00	0.001	0.002	0.003	0.025	0.013	0.008
15.00	0.003	0.012	0.016	0.185	0.056	0.051
20.00	0.009	0.031	0.040	0.623	0.125	0.186
25.00	0.019	0.061	0.080	1.516	0.242	0.479
30.00	0.034	0.104	0.138	3.130	0.412	1.016
35.00	0.054	0.164	0.218	5.723	0.634	1.897
40.00	0.081	0.239	0.319	9.548	0.904	3.230
45.00	0.114	0.330	0.444	14.835	1.218	5.128
50.00	0.154	0.436	0.590	21.792	1.571	7.703
55.00	0.201	0.557	0.758	30.611	1.967	11.063
60.00	0.255	0.693	0.949	41.599	2.445	15.319
65.00	0.317	0.849	1.166	55.190	3.001	20.594
70.00	0.386	1.024	1.410	71.684	3.602	27.023
75.00	0.463	1.217	1.680	91.255	4.230	34.737
80.00	0.548	1.425	1.974	114.02	4.883	43.861
85.00	0.641	1.649	2.290	140.14	5.567	54.511
90.00	0.742	1.886	2.628	169.73	6.273	66.797
95.00	0.851	2.136	2.986	202.89	6.992	80.825
100.00	0.967	2.397	3.364	239.66	7.717	96.693
105.00	1.090	2.667	3.758	280.06	8.445	114.49
110.00	1.221	2.946	4.167	324.11	9.174	134.30
115.00	1.358	3.233	4.591	371.81	9.906	156.19
120.00	1.502	3.526	5.028	423.18	10.642	180.23
125.00	1.652	3.826	5.477	478.20	11.365	206.49
130.00	1.808	4.129	5.937	536.82	12.081	235.02
135.00	1.969	4.437	6.406	598.99	12.785	265.88
140.00	2.136	4.747	6.884	664.64	13.475	299.10
145.00	2.308	5.060	7.369	733.71	14.150	334.73
150.00	2.485	5.374	7.859	806.12	14.810	372.80
155.00	2.667	5.689	8.356	881.78	15.454	413.33
160.00	2.852	6.004	8.856	960.63	16.083	456.36
165.00	3.042	6.319	9.361	1042.6	16.697	501.90
170.00	3.235	6.633	9.868	1127.6	17.295	549.97
175.00	3.432	6.946	10.378	1215.5	17.879	600.58
180.00	3.632	7.257	10.889	1306.3	18.448	653.75
185.00	3.835	7.567	11.402	1400.0	19.002	709.48
190.00	4.041	7.875	11.916	1496.3	19.543	767.77
195.00	4.249	8.181	12.431	1595.4	20.069	828.64
200.00	4.460	8.485	12.945	1697.0	20.581	892.08
205.00	4.674	8.786	13.460	1801.2	21.078	958.10
210.00	4.889	9.085	13.973	1907.8	21.561	1026.7
215.00	5.106	9.380	14.486	2016.7	22.031	1097.8
220.00	5.325	9.673	14.998	2128.0	22.488	1171.5
225.00	5.546	9.963	15.508	2241.6	22.933	1247.8
230.00	5.768	10.249	16.017	2357.3	23.366	1326.6
235.00	5.991	10.533	16.524	2475.2	23.790	1408.0
240.00	6.216	10.813	17.030	2595.2	24.203	1491.9
245.00	6.442	11.091	17.533	2717.3	24.607	1578.3
250.00	6.669	11.365	18.034	2841.3	25.004	1667.2
255.00	6.896	11.636	18.533	2967.3	25.393	1758.6
260.00	7.125	11.905	19.030	3095.2	25.776	1852.5
265.00	7.354	12.170	19.524	3225.0	26.150	1948.9
270.00	7.584	12.432	20.016	3356.7	26.515	2047.7
273.15	7.729	12.596	20.325	3440.6	26.738	2111.3
275.00	7.815	12.691	20.506	3490.1	26.867	2149.1
280.00	8.046	12.948	20.993	3625.3	27.205	2252.8
285.00	8.277	13.201	21.478	3762.2	27.528	2359.0
290.00	8.509	13.450	21.959	3900.6	27.837	2467.6
295.00	8.741	13.697	22.438	4040.5	28.134	2578.6
298.15	8.887	13.850	22.737	4129.4	28.318	2649.7
300.00	8.973	13.940	22.913	4181.9	28.425	2692.0

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-66(CONT.)

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM ORTHOSILICATE ($MG_2SI\ O_4$)
SOLID PHASE

GRAM MOLECULAR WT.=140.7076 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL / DEG MOLE	$(H_T^0-H_0^0)/T$ CAL / DEG MOLE	$(S_T^0-S_0^0)$ CAL / DEG MOLE	$(H_T^0-H_0^0)$ CAL / MOLE	C_P^0 CAL / DEG MOLE	$-(G_T^0-H_0^0)$ CAL / MOLE
300.00	8.973	13.940	22.913	4181.9	28.425	2692.0
310.00	9.438	14.416	23.854	4469.0	28.996	2925.8
320.00	9.903	14.881	24.784	4761.8	29.564	3169.0
330.00	10.368	15.334	25.702	5060.3	30.121	3421.4
340.00	10.832	15.777	26.609	5364.2	30.650	3683.0
350.00	11.296	16.209	27.505	5673.1	31.141	3953.6
360.00	11.758	16.630	28.389	5986.8	31.592	4233.1
370.00	12.220	17.040	29.260	6304.9	32.009	4521.3
373.15	12.365	17.167	29.532	6405.9	32.134	4613.9
380.00	12.680	17.439	30.119	6626.9	32.396	4818.2
390.00	13.138	17.827	30.965	6952.7	32.759	5123.6
400.00	13.594	18.205	31.799	7282.0	33.101	5437.5
425.00	14.725	19.105	33.829	8119.4	33.872	6258.0
450.00	15.841	19.944	35.785	8974.8	34.545	7128.3
475.00	16.940	20.728	37.669	9846.0	35.140	8046.6
500.00	18.022	21.463	39.485	10731.	35.671	9011.2
550.00	20.132	22.797	42.929	12539.	36.590	11073.
600.00	22.167	23.980	46.147	14388.	37.367	13300.
650.00	24.129	25.036	49.165	16274.	38.044	15684.
700.00	26.020	25.987	52.007	18191.	38.649	18214.
750.00	27.843	26.850	54.693	20137.	39.200	20882.
800.00	29.601	27.638	57.239	22110.	39.711	23681.
850.00	31.299	28.362	59.661	24108.	40.190	26604.
900.00	32.939	29.032	61.971	26129.	40.644	29645.
950.00	34.526	29.655	64.180	28172.	41.079	32799.
1000.00	36.062	30.237	66.298	30237.	41.498	36062.
1050.00	37.550	30.783	68.333	32322.	41.904	39428.
1100.00	38.994	31.297	70.291	34427.	42.300	42894.
1150.00	40.396	31.784	72.180	36551.	42.687	46456.
1200.00	41.759	32.246	74.005	38695.	43.066	50111.
1250.00	43.084	32.686	75.771	40858.	43.440	53855.
1300.00	44.374	33.107	77.481	43039.	43.808	57687.
1350.00	45.631	33.510	79.142	45239.	44.171	61602.
1400.00	46.857	33.897	80.755	47456.	44.531	65600.
1450.00	48.053	34.270	82.323	49692.	44.888	69677.
1500.00	49.221	34.630	83.851	51945.	45.241	73832.
1550.00	50.362	34.978	85.340	54216.	45.592	78062.
1600.00	51.478	35.315	86.793	56504.	45.941	82365.
1650.00	52.570	35.642	88.212	58810.	46.288	86740.
1700.00	53.639	35.961	89.599	61133.	46.633	91186.
1750.00	54.686	36.270	90.956	63473.	46.977	95700.
1800.00	55.712	36.573	92.284	65831.	47.319	100281.
1850.00	56.718	36.868	93.585	68205.	47.660	104928.
1900.00	57.705	37.156	94.861	70597.	48.000	109639.
1950.00	58.674	37.439	96.112	73005.	48.339	114413.
2000.00	59.625	37.715	97.340	75430.	48.677	119250.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-67

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM METATITANATE (MG TI O_3)
SOLID PHASE

T DEG K = 273.15 + T DEG C

GRAM MOLECULAR WT.=120.2102 GRAMS 1 1 CAL=4.1840 ABS J

T	$-(G^0_T-H^0_0)/T$	$(H^0_T-H^0_0)/T$	$(S^0_T-S^0_0)$	$(H^0_T-H^0_0)$	C^0_P	$-(G^0_T-H^0_0)$
DEG K	CAL/DEG MOLE	CAL/DEG MOLE	CAL/DEG MOLE	CAL/MOLE	CAL/DEG MOLE	CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.000	0.001	0.001	0.001
10.00	0.001	0.002	0.002	0.015	0.008	0.005
15.00	0.002	0.008	0.010	0.114	0.034	0.031
20.00	0.006	0.019	0.025	0.381	0.076	0.114
25.00	0.012	0.037	0.049	0.930	0.149	0.294
30.00	0.021	0.064	0.085	1.935	0.259	0.624
35.00	0.033	0.103	0.136	3.597	0.414	1.171
40.00	0.050	0.154	0.204	6.161	0.621	2.015
45.00	0.072	0.220	0.292	9.898	0.883	3.247
50.00	0.099	0.302	0.401	15.078	1.197	4.971
55.00	0.133	0.399	0.532	21.947	1.558	7.294
60.00	0.172	0.512	0.684	30.706	1.950	10.324
65.00	0.218	0.639	0.856	41.506	2.379	14.166
70.00	0.270	0.780	1.050	54.570	2.853	18.923
75.00	0.329	0.934	1.264	70.073	3.351	24.699
80.00	0.395	1.101	1.496	88.111	3.866	31.591
85.00	0.467	1.280	1.747	108.76	4.398	39.691
90.00	0.545	1.468	2.014	132.14	4.955	49.084
95.00	0.630	1.667	2.297	158.34	5.526	59.853
100.00	0.721	1.874	2.595	187.39	6.097	72.076
105.00	0.817	2.089	2.906	219.31	6.671	85.822
110.00	0.920	2.310	3.230	254.12	7.255	101.16
115.00	1.027	2.538	3.565	291.86	7.839	118.14
120.00	1.140	2.771	3.911	332.49	8.414	136.83
125.00	1.258	3.008	4.266	375.99	8.985	157.26
130.00	1.381	3.249	4.629	422.33	9.548	179.50
135.00	1.508	3.492	5.000	471.45	10.102	203.57
140.00	1.639	3.738	5.377	523.33	10.647	229.51
145.00	1.775	3.986	5.760	577.91	11.182	257.36
150.00	1.914	4.234	6.148	635.14	11.707	287.13
155.00	2.057	4.484	6.541	694.96	12.219	318.85
160.00	2.203	4.733	6.937	757.31	12.719	352.54
165.00	2.353	4.983	7.335	822.13	13.206	388.22
170.00	2.505	5.231	7.737	889.35	13.679	425.90
175.00	2.661	5.479	8.140	958.89	14.137	465.59
180.00	2.818	5.726	8.544	1030.7	14.580	507.30
185.00	2.979	5.971	8.950	1104.7	15.009	551.03
190.00	3.141	6.215	9.356	1180.8	15.426	596.80
195.00	3.306	6.456	9.762	1258.9	15.830	644.59
200.00	3.472	6.695	10.167	1339.0	16.222	694.41
205.00	3.640	6.932	10.573	1421.1	16.603	746.26
210.00	3.810	7.167	10.977	1505.1	16.972	800.13
215.00	3.982	7.399	11.381	1590.8	17.328	856.03
220.00	4.154	7.629	11.783	1678.3	17.671	913.94
225.00	4.328	7.856	12.184	1767.5	18.003	973.86
230.00	4.503	8.080	12.583	1858.3	18.326	1035.8
235.00	4.680	8.301	12.981	1950.7	18.641	1099.7
240.00	4.857	8.520	13.376	2044.7	18.952	1165.6
245.00	5.034	8.736	13.770	2140.2	19.258	1233.4
250.00	5.213	8.949	14.162	2237.3	19.558	1303.3
255.00	5.392	9.160	14.552	2335.8	19.852	1375.1
260.00	5.572	9.368	14.941	2435.8	20.135	1448.8
265.00	5.753	9.574	15.327	2537.2	20.407	1524.5
270.00	5.934	9.777	15.711	2639.8	20.665	1602.1
273.15	6.048	9.904	15.951	2705.2	20.821	1651.9
275.00	6.115	9.977	16.092	2743.8	20.910	1681.6
280.00	6.296	10.175	16.471	2848.9	21.145	1763.0
285.00	6.478	10.369	16.847	2955.2	21.373	1846.3
290.00	6.660	10.561	17.221	3062.6	21.598	1931.4
295.00	6.842	10.750	17.592	3171.[illegible]	21.82[illegible]	2018.5
298.15	6.957	10.868	17.825	3240.3	21.963	2074.3
300.00	7.025	10.936	17.961	3280.[illegible]	22.046	2107.4

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-67(CONT.)

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM METATITANATE (MG TI O_3)
SOLID PHASE

T DEG K = 273.15 + T DEG C

GRAM MOLECULAR WT.=120.2102 GRAMS 1 1 CAL=4.1840 ABS J

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
300.00	7.025	10.936	17.961	3280.9	22.046	2107.4
310.00	7.389	11.302	18.691	3503.6	22.498	2290.6
320.00	7.754	11.659	19.412	3730.8	22.942	2481.2
330.00	8.118	12.007	20.125	3962.4	23.363	2678.8
340.00	8.481	12.347	20.828	4198.0	23.752	2883.6
350.00	8.844	12.678	21.522	4437.3	24.108	3095.4
360.00	9.206	13.000	22.206	4680.0	24.434	3314.0
370.00	9.566	13.313	22.879	4925.9	24.735	3539.5
373.15	9.679	13.410	23.089	5003.9	24.826	3611.9
380.00	9.925	13.617	23.543	5174.6	25.015	3771.6
390.00	10.283	13.913	24.196	5426.1	25.276	4010.3
400.00	10.639	14.200	24.839	5680.1	25.521	4255.5
425.00	11.520	14.883	26.403	6325.1	26.068	4896.1
450.00	12.389	15.518	27.907	6982.9	26.541	5575.1
475.00	13.244	16.109	29.353	7651.7	26.954	6291.0
500.00	14.085	16.660	30.745	8330.2	27.318	7042.3
550.00	15.720	17.658	33.379	9712.0	27.935	8646.2
600.00	17.295	18.536	35.832	11122.	28.444	10377.
650.00	18.810	19.316	38.126	12555.	28.876	12227.
700.00	20.268	20.012	40.280	14009.	29.253	14187.
750.00	21.670	20.640	42.310	15480.	29.589	16252.
800.00	23.020	21.209	44.229	16967.	29.894	18416.
850.00	24.322	21.728	46.050	18469.	30.174	20674.
900.00	25.577	22.205	47.782	19984.	30.436	23020.
950.00	26.790	22.645	49.435	21513.	30.682	25450.
1000.00	27.962	23.053	51.014	23053.	30.917	27962.
1050.00	29.096	23.432	52.528	24604.	31.142	30551.
1100.00	30.194	23.788	53.982	26167.	31.358	33214.
1150.00	31.259	24.122	55.381	27740.	31.568	35948.
1200.00	32.293	24.436	56.729	29323.	31.772	38751.
1250.00	33.296	24.734	58.030	30917.	31.972	41620.
1300.00	34.272	25.016	59.287	32520.	32.168	44553.
1350.00	35.221	25.284	60.505	34134.	32.360	47548.
1400.00	36.145	25.540	61.685	35756.	32.549	50603.
1450.00	37.046	25.785	62.831	37388.	32.735	53716.
1500.00	37.924	26.020	63.944	39030.	32.920	56886.
1550.00	38.781	26.245	65.026	40680.	33.102	60110.
1600.00	39.617	26.463	66.080	42340.	33.283	63388.
1650.00	40.435	26.672	67.107	44009.	33.462	66718.
1700.00	41.234	26.874	68.108	45686.	33.640	70098.
1750.00	42.016	27.070	69.086	47373.	33.817	73528.
1800.00	42.781	27.260	70.041	49068.	33.992	77006.
1850.00	43.531	27.444	70.975	50772.	34.167	80532.
1900.00	44.265	27.623	71.888	52485.	34.341	84103.
1950.00	44.985	27.798	72.783	54206.	34.514	87720.
2000.00	45.691	27.968	73.659	55936.	34.687	91381.

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-68

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM DITITANATE (MG TI_2O_5)
SOLID PHASE

GRAM MOLECULAR WT.=200.1090 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG-MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG-MOLE	$(S^0_T-S^0_0)$ CAL/DEG-MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG-MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.001	0.003	0.002	0.002
10.00	0.002	0.005	0.007	0.050	0.025	0.017
15.00	0.007	0.025	0.032	0.371	0.112	0.102
20.00	0.019	0.062	0.081	1.244	0.248	0.372
25.00	0.038	0.120	0.158	3.005	0.472	0.957
30.00	0.067	0.203	0.270	6.099	0.777	2.014
35.00	0.106	0.311	0.417	10.887	1.148	3.720
40.00	0.156	0.442	0.598	17.682	1.579	6.244
45.00	0.217	0.595	0.812	26.784	2.072	9.756
50.00	0.288	0.770	1.059	38.522	2.635	14.419
55.00	0.371	0.969	1.339	53.269	3.278	20.401
60.00	0.465	1.191	1.656	71.471	4.021	27.873
65.00	0.570	1.440	2.010	93.614	4.843	37.021
70.00	0.686	1.713	2.399	119.92	5.680	48.030
75.00	0.814	2.006	2.820	150.43	6.526	61.066
80.00	0.953	2.316	3.269	185.25	7.408	76.277
85.00	1.104	2.642	3.745	224.54	8.309	93.802
90.00	1.264	2.982	4.246	268.34	9.213	113.77
95.00	1.435	3.333	4.768	316.68	10.120	136.30
100.00	1.615	3.695	5.310	369.54	11.025	161.48
105.00	1.804	4.066	5.870	426.93	11.930	189.43
110.00	2.002	4.444	6.446	488.84	12.837	220.21
115.00	2.208	4.829	7.037	555.29	13.742	253.91
120.00	2.422	5.219	7.640	626.24	14.632	290.60
125.00	2.643	5.613	8.255	701.59	15.509	330.33
130.00	2.871	6.010	8.881	781.30	16.370	373.17
135.00	3.105	6.409	9.514	865.27	17.214	419.15
140.00	3.345	6.810	10.155	953.41	18.040	468.32
145.00	3.591	7.211	10.802	1045.6	18.846	520.72
150.00	3.842	7.612	11.455	1141.8	19.631	576.36
155.00	4.099	8.012	12.111	1241.9	20.397	635.27
160.00	4.359	8.411	12.770	1345.8	21.143	697.47
165.00	4.624	8.808	13.432	1453.3	21.870	762.97
170.00	4.893	9.203	14.095	1564.4	22.578	831.79
175.00	5.165	9.595	14.760	1679.1	23.267	903.93
180.00	5.441	9.984	15.425	1797.1	23.936	979.39
185.00	5.720	10.370	16.090	1918.4	24.585	1058.2
190.00	6.002	10.752	16.754	2042.9	25.215	1140.3
195.00	6.286	11.131	17.416	2170.5	25.826	1225.7
200.00	6.572	11.506	18.078	2301.1	26.418	1314.4
205.00	6.861	11.876	18.737	2434.6	26.993	1406.5
210.00	7.152	12.243	19.394	2571.0	27.554	1501.8
215.00	7.444	12.605	20.049	2710.2	28.099	1600.4
220.00	7.738	12.964	20.701	2852.0	28.629	1702.3
225.00	8.033	13.317	21.350	2996.4	29.143	1807.4
230.00	8.330	13.667	21.996	3143.4	29.640	1915.8
235.00	8.627	14.012	22.639	3292.8	30.120	2027.4
240.00	8.926	14.352	23.278	3444.6	30.583	2142.2
245.00	9.225	14.688	23.913	3598.6	31.031	2260.2
250.00	9.525	15.019	24.545	3754.8	31.466	2381.3
255.00	9.826	15.346	25.172	3913.2	31.891	2505.6
260.00	10.127	15.668	25.795	4073.7	32.306	2633.0
265.00	10.429	15.986	26.415	4236.3	32.714	2763.6
270.00	10.730	16.299	27.030	4400.9	33.113	2897.2
273.15	10.920	16.495	27.415	4505.6	33.359	2982.9
275.00	11.032	16.609	27.641	4567.4	33.502	3033.8
280.00	11.334	16.914	28.248	4735.9	33.881	3173.6
285.00	11.636	17.215	28.851	4906.2	34.247	3316.3
290.00	11.938	17.511	29.450	5078.3	34.601	3462.1
295.00	12.240	17.804	30.044	5252.2	34.940	3610.8
298.15	12.430	17.986	30.416	5362.6	35.147	3706.0
300.00	12.542	18.092	30.634	5427.7	35.266	3762.5

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-68(CONT.)

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM DITITANATE (MG TI_2O_5)
SOLID PHASE

GRAM MOLECULAR WT.=200.1090 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
300.00	12.542	18.092	30.634	5427.7	35.266	3762.5
310.00	13.144	18.656	31.800	5783.5	35.879	4074.7
320.00	13.745	19.203	32.949	6145.1	36.445	4398.5
330.00	14.344	19.734	34.078	6512.2	36.968	4733.6
340.00	14.941	20.248	35.189	6884.3	37.452	5080.0
350.00	15.535	20.746	36.281	7261.1	37.902	5437.3
360.00	16.126	21.229	37.355	7642.3	38.322	5805.5
370.00	16.714	21.696	38.410	8027.5	38.716	6184.4
373.15	16.899	21.840	38.739	8149.6	38.835	6305.9
380.00	17.299	22.149	39.448	8416.5	39.086	6573.7
390.00	17.880	22.588	40.468	8809.1	39.436	6973.3
400.00	18.457	23.013	41.470	9205.2	39.766	7383.0
425.00	19.883	24.021	43.904	10209.	40.520	8450.4
450.00	21.283	24.957	46.240	11230.	41.190	9577.3
475.00	22.656	25.827	48.483	12268.	41.792	10762.
500.00	24.002	26.639	50.641	13320.	42.339	12001.
550.00	26.611	28.112	54.723	15461.	43.310	14636.
600.00	29.114	29.414	58.528	17649.	44.158	17468.
650.00	31.515	30.578	62.093	19876.	44.920	20485.
700.00	33.820	31.628	65.448	22140.	45.620	23674.
750.00	36.035	32.583	68.618	24437.	46.273	27026.
800.00	38.166	33.458	71.624	26767.	46.892	30533.
850.00	40.219	34.266	74.485	29126.	47.483	34186.
900.00	42.199	35.016	77.215	31515.	48.053	37979.
950.00	44.111	35.717	79.828	33931.	48.606	41906.
1000.00	45.960	36.375	82.335	36375.	49.145	45960.
1050.00	47.750	36.996	84.746	38845.	49.673	50137.
1100.00	49.485	37.584	87.068	41342.	50.193	54433.
1150.00	51.168	38.143	89.311	43865.	50.704	58843.
1200.00	52.802	38.677	91.480	46412.	51.210	63363.
1250.00	54.392	39.188	93.580	48985.	51.710	67990.
1300.00	55.938	39.680	95.618	51583.	52.205	72720.
1350.00	57.445	40.153	97.597	54206.	52.697	77551.
1400.00	58.913	40.609	99.523	56853.	53.185	82479.
1450.00	60.346	41.051	101.40	59524.	53.670	87502.
1500.00	61.745	41.480	103.23	62220.	54.153	92618.
1550.00	63.112	41.897	105.01	64940.	54.634	97824.
1600.00	64.449	42.302	106.75	67683.	55.113	103118.
1650.00	65.756	42.698	108.45	70451.	55.590	108498.
1700.00	67.037	43.084	110.12	73242.	56.066	113963.
1750.00	68.291	43.461	111.75	76057.	56.540	119510.
1800.00	69.521	43.831	113.35	78896.	57.013	125137.
1850.00	70.727	44.194	114.92	81759.	57.485	130844.
1900.00	71.910	44.550	116.46	84645.	57.956	136629.
1950.00	73.072	44.900	117.97	87554.	58.427	142490.
2000.00	74.213	45.244	119.46	90487.	58.896	148426.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-69

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM ORTHOTITANATE ($MG_2TI\ O_4$)
SOLID PHASE

GRAM MOLECULAR WT.=160.5216 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
0.	1.378	0.000	1.378	0.000	0.000	0.000
5.00	1.378	0.000	1.378	0.001	0.001	6.890
10.00	1.379	0.003	1.381	0.026	0.013	13.787
15.00	1.381	0.013	1.394	0.196	0.059	20.721
20.00	1.388	0.033	1.420	0.654	0.131	27.753
25.00	1.398	0.064	1.462	1.592	0.254	34.950
30.00	1.413	0.110	1.523	3.287	0.433	42.403
35.00	1.435	0.172	1.607	6.015	0.668	50.218
40.00	1.463	0.252	1.714	10.061	0.960	58.510
45.00	1.498	0.349	1.847	15.712	1.311	67.402
50.00	1.540	0.465	2.006	23.272	1.722	77.023
55.00	1.591	0.600	2.191	33.005	2.178	87.505
60.00	1.650	0.753	2.402	45.161	2.699	98.977
65.00	1.717	0.925	2.642	60.133	3.299	111.58
70.00	1.792	1.117	2.909	78.191	3.927	125.44
75.00	1.876	1.326	3.202	99.436	4.578	140.71
80.00	1.969	1.551	3.519	124.06	5.278	157.50
85.00	2.070	1.791	3.861	152.26	6.004	175.94
90.00	2.179	2.046	4.225	184.13	6.750	196.15
95.00	2.297	2.314	4.611	219.78	7.511	218.23
100.00	2.423	2.593	5.015	259.25	8.279	242.29
105.00	2.556	2.882	5.438	302.59	9.058	268.42
110.00	2.697	3.180	5.878	349.85	9.851	296.70
115.00	2.845	3.488	6.334	401.15	10.674	327.22
120.00	3.001	3.806	6.806	456.69	11.554	360.06
125.00	3.162	4.131	7.293	516.37	12.325	395.31
130.00	3.331	4.461	7.792	579.98	13.118	433.02
135.00	3.506	4.796	8.302	647.50	13.886	473.25
140.00	3.686	5.134	8.820	718.79	14.630	516.05
145.00	3.872	5.474	9.347	793.80	15.371	561.46
150.00	4.064	5.816	9.880	872.47	16.0[illegible]7	609.53
155.00	4.260	6.160	10.420	954.75	16.813	660.27
160.00	4.461	6.504	10.965	1040.6	17.519	713.73
165.00	4.666	6.848	11.514	1129.9	18.209	769.93
170.00	4.876	7.192	12.068	1222.7	18.885	828.88
175.00	5.089	7.536	12.625	1318.7	19.541	890.61
180.00	5.306	7.878	13.184	1418.0	20.178	955.13
185.00	5.527	8.219	13.746	1520.5	20.796	1022.5
190.00	5.750	8.558	14.308	1626.0	21.394	1092.6
195.00	5.977	8.894	14.871	1734.4	21.976	1165.5
200.00	6.207	9.228	15.435	1845.7	22.543	1241.3
205.00	6.438	9.560	15.998	1959.8	23.095	1319.9
210.00	6.673	9.889	16.561	2076.6	23.632	1401.3
215.00	6.909	10.214	17.124	2196.1	24.155	1485.5
220.00	7.148	10.537	17.685	2318.1	24.661	1572.5
225.00	7.388	10.856	18.245	2442.7	25.149	1662.3
230.00	7.630	11.172	18.802	2569.6	25.620	1755.0
235.00	7.874	11.484	19.358	2698.8	26.073	1850.4
240.00	8.119	11.793	19.912	2830.3	26.510	1948.5
245.00	8.365	12.098	20.463	2963.9	26.934	2049.5
250.00	8.613	12.398	21.011	3099.6	27.345	2153.2
255.00	8.861	12.696	21.557	3237.4	27.746	2259.6
260.00	9.111	12.989	22.099	3377.1	28.138	2368.7
265.00	9.361	13.278	22.639	3518.7	28.519	2480.6
270.00	9.612	13.564	23.175	3662.2	28.889	2595.1
273.15	9.770	13.742	23.512	3753.6	29.116	2668.6
275.00	9.863	13.846	23.709	3807.6	29.247	2712.3
280.00	10.115	14.124	24.239	3954.7	29.593	2832.2
285.00	10.367	14.398	24.766	4103.5	29.926	2954.7
290.00	10.620	14.669	25.289	4253.9	30.248	3079.8
295.00	10.873	14.935	25.809	4406.0	30.558	3207.6
298.15	11.033	15.101	26.134	4502.5	30.748	3289.4
300.00	11.126	15.198	26.325	4559.5	30.858	3337.9

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-69(CONT.)

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM ORTHOTITANATE ($MG_2TI\ O_4$)
SOLID PHASE

GRAM MOLECULAR WT.=160.5216 GRAMS　　　1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
300.00	11.126	15.198	26.325	4559.5	30.858	3337.9
310.00	11.633	15.713	27.346	4871.0	31.428	3606.3
320.00	12.140	16.212	28.352	5187.9	31.959	3884.8
330.00	12.646	16.697	29.343	5510.0	32.451	4173.3
340.00	13.152	17.167	30.319	5836.8	32.905	4471.6
350.00	13.656	17.623	31.279	6168.0	33.326	4779.6
360.00	14.159	18.065	32.223	6503.2	33.719	5097.1
370.00	14.660	18.493	33.152	6842.3	34.088	5424.0
373.15	14.817	18.625	33.442	6949.9	34.199	5528.9
380.00	15.158	18.908	34.066	7184.9	34.434	5760.1
390.00	15.655	19.310	34.965	7530.9	34.761	6105.3
400.00	16.148	19.700	35.849	7880.1	35.070	6459.4
425.00	17.371	20.625	37.996	8765.8	35.775	7382.6
450.00	18.574	21.485	40.059	9668.2	36.400	8358.5
475.00	19.758	22.285	42.043	10585.	36.963	9384.9
500.00	20.920	23.032	43.952	11516.	37.473	10460.
550.00	23.180	24.387	47.567	13413.	38.379	12749.
600.00	25.354	25.586	50.941	15352.	39.170	15213.
650.00	27.446	26.659	54.105	17328.	39.880	17840.
700.00	29.457	27.627	57.084	19339.	40.532	20620.
750.00	31.393	28.508	59.901	21381.	41.140	23545.
800.00	33.259	29.316	62.575	23452.	41.715	26608.
850.00	35.059	30.061	65.121	25552.	42.265	29800.
900.00	36.797	30.754	67.552	27679.	42.795	33118.
950.00	38.478	31.401	69.879	29831.	43.310	36554.
1000.00	40.104	32.009	72.113	32009.	43.811	40104.
1050.00	41.680	32.583	74.263	34212.	44.302	43764.
1100.00	43.208	33.127	76.335	36439.	44.785	47529.
1150.00	44.692	33.644	78.336	38691.	45.260	51396.
1200.00	46.135	34.138	80.272	40965.	45.729	55362.
1250.00	47.538	34.611	82.149	43263.	46.194	59422.
1300.00	48.904	35.065	83.969	45585.	46.654	63576.
1350.00	50.236	35.503	85.739	47929.	47.111	67818.
1400.00	51.535	35.926	87.460	50296.	47.564	72149.
1450.00	52.803	36.335	89.137	52685.	48.015	76564.
1500.00	54.041	36.731	90.773	55097.	48.464	81062.
1550.00	55.252	37.117	92.369	57532.	48.910	85640.
1600.00	56.436	37.493	93.929	59988.	49.355	90298.
1650.00	57.596	37.859	95.454	62467.	49.798	95033.
1700.00	58.731	38.216	96.947	64968.	50.240	99843.
1750.00	59.844	38.566	98.410	67491.	50.680	104727.
1800.00	60.935	38.909	99.844	70036.	51.119	109683.
1850.00	62.006	39.245	101.25	72603.	51.558	114711.
1900.00	63.057	39.575	102.63	75192.	51.995	119808.
1950.00	64.089	39.899	103.99	77802.	52.432	124973.
2000.00	65.103	40.217	105.32	80435.	52.868	130206.

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-70

THERMODYNAMIC FUNCTIONS FOR LEAD (PB)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=207.19 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ $\frac{\text{CAL}}{\text{DEG MOLE}}$	$(H_T^0-H_0^0)/T$ $\frac{\text{CAL}}{\text{DEG MOLE}}$	$(S_T^0-S_0^0)$ $\frac{\text{CAL}}{\text{DEG MOLE}}$	$(H_T^0-H_0^0)$ $\frac{\text{CAL}}{\text{MOLE}}$	C_P^0 $\frac{\text{CAL}}{\text{DEG MOLE}}$	$-(G_T^0-H_0^0)$ $\frac{\text{CAL}}{\text{MOLE}}$
SOLID PHASE						
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.014	0.023	0.038	0.116	0.079	0.072
10.00	0.064	0.170	0.234	1.697	0.663	0.644
15.00	0.191	0.500	0.691	7.507	1.680	2.859
20.00	0.390	0.911	1.302	18.229	2.579	7.807
25.00	0.638	1.326	1.965	33.161	3.370	15.961
30.00	0.915	1.717	2.632	51.512	3.938	27.462
35.00	1.207	2.068	3.274	72.365	4.381	42.242
40.00	1.504	2.376	3.880	95.056	4.675	60.146
45.00	1.799	2.645	4.444	119.02	4.906	80.973
50.00	2.091	2.882	4.973	144.10	5.122	104.53
55.00	2.375	3.093	5.468	170.09	5.260	130.64
60.00	2.653	3.278	5.930	196.68	5.385	159.15
65.00	2.922	3.446	6.368	223.99	5.526	189.91
70.00	3.183	3.596	6.779	251.74	5.566	222.78
75.00	3.435	3.729	7.164	279.68	5.611	257.65
80.00	3.680	3.848	7.528	307.84	5.655	294.39
85.00	3.916	3.956	7.872	336.24	5.706	332.90
90.00	4.145	4.054	8.199	364.86	5.736	373.09
95.00	4.367	4.143	8.510	393.63	5.780	414.87
100.00	4.582	4.227	8.809	422.70	5.847	458.17
105.00	4.790	4.305	9.095	452.04	5.886	502.93
110.00	4.992	4.378	9.369	481.54	5.913	549.10
115.00	5.188	4.445	9.633	511.15	5.923	596.61
120.00	5.378	4.506	9.885	540.78	5.938	645.41
125.00	5.564	4.564	10.128	570.52	5.958	695.44
130.00	5.744	4.618	10.362	600.35	5.975	746.67
135.00	5.919	4.669	10.588	630.27	5.994	799.04
140.00	6.090	4.716	10.806	660.28	6.012	852.53
145.00	6.256	4.761	11.017	690.39	6.029	907.09
150.00	6.418	4.804	11.222	720.57	6.044	962.69
155.00	6.576	4.844	11.420	750.82	6.058	1019.3
160.00	6.731	4.882	11.613	781.15	6.071	1076.9
165.00	6.881	4.918	11.800	811.53	6.083	1135.4
170.00	7.029	4.953	11.981	841.97	6.094	1194.9
175.00	7.173	4.986	12.158	872.47	6.106	1255.2
180.00	7.314	5.017	12.330	903.03	6.117	1316.4
185.00	7.451	5.047	12.498	933.65	6.129	1378.5
190.00	7.586	5.075	12.662	964.32	6.141	1441.4
195.00	7.719	5.103	12.821	995.06	6.153	1505.1
200.00	7.848	5.129	12.977	1025.9	6.165	1569.6
205.00	7.975	5.155	13.130	1056.7	6.177	1634.9
210.00	8.100	5.179	13.279	1087.6	6.188	1700.9
215.00	8.222	5.203	13.424	1118.6	6.199	1767.7
220.00	8.342	5.225	13.567	1149.6	6.210	1835.2
225.00	8.459	5.247	13.707	1180.7	6.221	1903.3
230.00	8.575	5.269	13.844	1211.8	6.231	1972.2
235.00	8.688	5.289	13.978	1243.0	6.241	2041.8
240.00	8.800	5.309	14.109	1274.2	6.251	2112.0
245.00	8.910	5.329	14.238	1305.5	6.260	2182.9
250.00	9.017	5.347	14.365	1336.8	6.270	2254.4
255.00	9.124	5.365	14.489	1368.2	6.279	2326.5
260.00	9.228	5.383	14.611	1399.6	6.288	2399.3
265.00	9.331	5.400	14.731	1431.1	6.297	2472.6
270.00	9.432	5.417	14.849	1462.6	6.306	2546.6
273.15	9.495	5.427	14.922	1482.5	6.311	2593.5
275.00	9.531	5.433	14.964	1494.1	6.315	2621.1
280.00	9.629	5.449	15.078	1525.7	6.324	2696.2
285.00	9.726	5.464	15.190	1557.4	6.333	2771.9
290.00	9.821	5.479	15.301	1589.1	6.342	2848.1
295.00	9.915	5.494	15.409	1620.8	6.351	2924.9
298.15	9.973	5.503	15.477	1640.8	6.357	2973.5
300.00	10.007	5.509	15.516	1652.6	6.360	3002.2

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-70(CONT.)

THERMODYNAMIC FUNCTIONS FOR LEAD (PB)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=207.19 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
SOLID PHASE						
300.00	10.007	5.509	15.516	1652.6	6.360	3002.2
310.00	10.188	5.536	15.725	1716.3	6.379	3158.4
320.00	10.365	5.563	15.928	1780.2	6.399	3316.7
330.00	10.536	5.589	16.125	1844.2	6.418	3476.9
340.00	10.703	5.613	16.317	1908.5	6.438	3639.1
350.00	10.866	5.637	16.504	1973.0	6.458	3803.3
360.00	11.026	5.660	16.686	2037.7	6.478	3969.2
370.00	11.181	5.683	16.864	2102.6	6.498	4137.0
373.15	11.229	5.689	16.919	2123.0	6.504	4190.2
380.00	11.333	5.704	17.037	2167.6	6.518	4306.5
390.00	11.481	5.725	17.207	2232.9	6.539	4477.7
400.00	11.626	5.746	17.372	2298.4	6.560	4650.6
425.00	11.976	5.796	17.772	2463.1	6.617	5089.9
450.00	12.309	5.843	18.152	2629.3	6.675	5539.0
475.00	12.626	5.888	18.514	2796.9	6.733	5997.4
500.00	12.929	5.932	18.861	2965.9	6.791	6464.6
550.00	13.498	6.015	19.514	3308.4	6.908	7424.2
600.00	14.025	6.095	20.120	3656.7	7.024	8415.2
600.60	14.031	6.095	20.127	3660.9	7.025	8427.3
LIQUID PHASE						
600.60	14.031	7.992	22.024	4800.0	7.315	8427.3
650.00	14.661	7.939	22.600	5160.5	7.279	9529.8
700.00	15.248	7.891	23.138	5523.5	7.242	10673.
750.00	15.791	7.846	23.637	5884.7	7.206	11843.
800.00	16.296	7.805	24.101	6244.0	7.169	13037.
850.00	16.768	7.767	24.534	6601.6	7.133	14253.
900.00	17.211	7.730	24.941	6957.3	7.096	15490.
950.00	17.628	7.696	25.324	7311.2	7.060	16746.
1000.00	18.022	7.663	25.685	7663.3	7.023	18022.
1050.00	18.395	7.632	26.027	8013.5	6.987	19314.
1100.00	18.749	7.602	26.351	8362.0	6.950	20624.
1150.00	19.086	7.573	26.659	8708.6	6.914	21949.
1200.00	19.408	7.544	26.952	9053.3	6.877	23290.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-71

THERMODYNAMIC FUNCTIONS FOR YELLOW LEAD MONOXIDE (PB O)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=223.1894 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
			SOLID PHASE			
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.002	0.003	0.005	0.014	0.009	0.010
10.00	0.009	0.028	0.037	0.283	0.154	0.088
15.00	0.041	0.167	0.208	2.504	0.783	0.620
20.00	0.120	0.392	0.512	7.845	1.344	2.391
25.00	0.234	0.643	0.877	16.079	1.954	5.838
30.00	0.374	0.906	1.281	27.195	2.467	11.224
35.00	0.533	1.163	1.696	40.706	2.944	18.662
40.00	0.705	1.414	2.119	56.569	3.381	28.199
45.00	0.886	1.654	2.540	74.441	3.773	39.848
50.00	1.072	1.885	2.957	94.263	4.136	53.593
55.00	1.262	2.103	3.365	115.65	4.422	69.402
60.00	1.454	2.308	3.762	138.49	4.705	87.223
65.00	1.646	2.502	4.148	162.62	4.949	107.00
70.00	1.838	2.686	4.525	188.04	5.219	128.69
75.00	2.030	2.863	4.893	214.75	5.460	152.24
80.00	2.220	3.033	5.253	242.63	5.696	177.60
85.00	2.409	3.197	5.606	271.75	5.956	204.75
90.00	2.596	3.358	5.954	302.19	6.208	233.66
95.00	2.782	3.512	6.294	333.68	6.390	264.28
100.00	2.966	3.662	6.628	366.17	6.605	296.59
105.00	3.148	3.807	6.955	399.70	6.809	330.54
110.00	3.328	3.948	7.276	434.26	7.009	366.12
115.00	3.507	4.085	7.592	469.74	7.185	403.30
120.00	3.684	4.218	7.901	506.14	7.381	442.03
125.00	3.858	4.348	8.206	543.50	7.559	482.30
130.00	4.031	4.475	8.506	581.73	7.736	524.09
135.00	4.203	4.599	8.802	620.85	7.911	567.36
140.00	4.372	4.720	9.092	660.83	8.079	612.09
145.00	4.540	4.839	9.379	701.63	8.243	658.27
150.00	4.706	4.955	9.661	743.24	8.400	705.87
155.00	4.870	5.069	9.939	785.62	8.550	754.87
160.00	5.033	5.180	10.212	828.73	8.693	805.25
165.00	5.194	5.288	10.482	872.54	8.827	856.99
170.00	5.353	5.394	10.747	916.99	8.953	910.07
175.00	5.511	5.497	11.009	962.05	9.071	964.46
180.00	5.667	5.598	11.266	1007.7	9.183	1020.1
185.00	5.822	5.697	11.519	1053.9	9.289	1077.1
190.00	5.975	5.792	11.768	1100.6	9.389	1135.3
195.00	6.127	5.886	12.013	1147.8	9.486	1194.8
200.00	6.277	5.977	12.254	1195.4	9.577	1255.5
205.00	6.426	6.066	12.492	1243.5	9.665	1317.3
210.00	6.573	6.153	12.726	1292.1	9.750	1380.4
215.00	6.719	6.237	12.956	1341.0	9.834	1444.6
220.00	6.863	6.320	13.183	1390.4	9.917	1509.9
225.00	7.006	6.401	13.407	1440.2	10.001	1576.4
230.00	7.148	6.480	13.628	1490.4	10.085	1644.0
235.00	7.288	6.558	13.846	1541.0	10.169	1712.7
240.00	7.427	6.634	14.061	1592.1	10.250	1782.4
245.00	7.564	6.708	14.273	1643.5	10.327	1853.3
250.00	7.701	6.781	14.482	1695.4	10.400	1925.2
255.00	7.836	6.853	14.689	1747.5	10.467	1998.1
260.00	7.969	6.923	14.893	1800.0	10.529	2072.0
265.00	8.102	6.992	15.094	1852.8	10.588	2147.0
270.00	8.233	7.059	15.292	1905.9	10.644	2223.0
273.15	8.315	7.100	15.416	1939.5	10.679	2271.3
275.00	8.363	7.125	15.488	1959.2	10.699	2299.9
280.00	8.492	7.189	15.681	2012.9	10.753	2377.8
285.00	8.620	7.252	15.872	2066.8	10.806	2456.7
290.00	8.747	7.314	16.060	2120.9	10.857	2536.6
295.00	8.872	7.374	16.246	2175.3	10.907	2617.3
298.15	8.951	7.412	16.362	2209.7	10.938	2668.7
300.00	8.997	7.433	16.430	2230.0	10.955	2699.0

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-71(CONT.)

THERMODYNAMIC FUNCTIONS FOR YELLOW LEAD MONOXIDE (PB O)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=223.1894 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
			SOLID PHASE			
300.00	8.997	7.433	16.430	2230.0	10.955	2699.0
310.00	9.242	7.548	16.791	2340.0	11.044	2865.1
320.00	9.484	7.659	17.143	2450.9	11.124	3034.8
330.00	9.721	7.765	17.486	2562.4	11.195	3208.0
340.00	9.954	7.867	17.821	2674.7	11.261	3384.5
350.00	10.184	7.965	18.149	2787.7	11.326	3564.4
360.00	10.410	8.059	18.469	2901.2	11.389	3747.4
370.00	10.632	8.150	18.781	3015.4	11.451	3933.7
373.15	10.701	8.178	18.879	3051.5	11.470	3993.0
380.00	10.850	8.237	19.088	3130.2	11.511	4123.1
390.00	11.065	8.322	19.387	3245.7	11.571	4315.4
400.00	11.277	8.404	19.681	3361.7	11.629	4510.8
450.00	12.289	8.777	21.065	3949.5	11.877	5529.9
500.00	13.230	9.098	22.328	4548.9	12.093	6615.2
550.00	14.111	9.379	23.490	5158.5	12.288	7761.1
600.00	14.938	9.629	24.567	5777.4	12.468	8962.8
650.00	15.718	9.854	25.572	6405.1	12.639	10217.
700.00	16.456	10.059	26.514	7041.2	12.802	11519.
750.00	17.156	10.247	27.403	7685.3	12.960	12867.
800.00	17.823	10.421	28.245	8337.2	13.115	14259.
850.00	18.460	10.584	29.044	8996.7	13.265	15691.
900.00	19.069	10.737	29.807	9663.6	13.414	17162.
950.00	19.654	10.882	30.536	10338.	13.560	18671.
1000.00	20.215	11.020	31.235	11020.	13.706	20215.
1050.00	20.756	11.151	31.907	11709.	13.849	21794.
1100.00	21.278	11.277	32.555	12405.	13.991	23406.
1150.00	21.782	11.398	33.180	13108.	14.133	25049.
1170.00	21.979	11.445	33.424	13391.	14.190	25715.
			LIQUID PHASE			
1170.00	21.979	16.512	38.491	19319.	23.899	25715.
1200.00	22.400	16.696	39.096	20036.	23.899	26880.
1250.00	23.090	16.985	40.075	21231.	23.899	28862.
1300.00	23.763	17.251	41.014	22426.	23.899	30892.
1350.00	24.420	17.497	41.917	23621.	23.899	32967.
1400.00	25.062	17.725	42.787	24816.	23.899	35087.
1450.00	25.689	17.938	43.627	26011.	23.899	37249.
1500.00	26.302	18.137	44.439	27205.	23.899	39453.
1550.00	26.901	18.323	45.224	28400.	23.899	41696.
1600.00	27.486	18.497	45.983	29595.	23.899	43978.
1650.00	28.059	18.661	46.720	30790.	23.899	46298.
1700.00	28.620	18.815	47.435	31985.	23.899	48653.
1750.00	29.168	18.960	48.128	33180.	23.899	51044.
1800.00	29.705	19.097	18.802	34375.	23.899	53469.
1850.00	30.231	19.227	49.458	35570.	23.899	55927.
1900.00	30.746	19.350	50.096	36765.	23.899	58417.
1950.00	31.251	19.467	50.718	37960.	23.899	60939.
2000.00	31.746	19.577	51.323	39155.	23.899	63492.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-72

THERMODYNAMIC FUNCTIONS FOR RED LEAD MONOXIDE (PB O)
SOLID PHASE

GRAM MOLECULAR WT.=223.1894 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.002	0.002	0.004	0.012	0.007	0.008
10.00	0.007	0.020	0.027	0.204	0.101	0.068
15.00	0.027	0.097	0.124	1.448	0.427	0.405
20.00	0.072	0.233	0.305	4.650	0.877	1.444
25.00	0.143	0.418	0.562	10.461	1.461	3.579
30.00	0.239	0.643	0.881	19.278	2.061	7.166
35.00	0.356	0.885	1.241	30.983	2.611	12.460
40.00	0.490	1.132	1.622	45.275	3.094	19.613
45.00	0.638	1.374	2.011	61.808	3.510	28.695
50.00	0.794	1.606	2.400	80.286	3.874	39.725
55.00	0.958	1.827	2.785	100.46	4.186	52.690
60.00	1.126	2.035	3.161	122.08	4.460	67.556
65.00	1.297	2.232	3.528	145.06	4.731	84.282
70.00	1.469	2.420	3.889	169.39	4.999	102.83
75.00	1.642	2.600	4.243	195.03	5.256	123.16
80.00	1.816	2.774	4.589	221.92	5.497	145.24
85.00	1.989	2.941	4.930	249.99	5.732	169.04
90.00	2.161	3.103	5.264	279.24	5.965	194.53
95.00	2.333	3.259	5.593	309.64	6.195	221.67
100.00	2.504	3.412	5.916	341.18	6.421	250.45
105.00	2.675	3.560	6.235	373.84	6.639	280.83
110.00	2.844	3.705	6.549	407.55	6.847	312.79
115.00	3.011	3.846	6.857	442.29	7.048	346.31
120.00	3.178	3.984	7.162	478.03	7.245	381.35
125.00	3.343	4.118	7.461	514.74	7.440	417.91
130.00	3.507	4.249	7.757	552.41	7.628	455.96
135.00	3.670	4.378	8.048	591.01	7.810	495.47
140.00	3.832	4.504	8.335	630.50	7.986	536.43
145.00	3.992	4.627	8.618	670.85	8.154	578.82
150.00	4.151	4.747	8.898	712.03	8.314	622.61
155.00	4.308	4.864	9.173	753.98	8.467	667.79
160.00	4.465	4.979	9.444	796.68	8.612	714.33
165.00	4.620	5.091	9.711	840.10	8.751	762.22
170.00	4.773	5.201	9.974	884.18	8.883	811.44
175.00	4.925	5.308	10.234	928.92	9.009	861.96
180.00	5.076	5.413	10.489	974.27	9.130	913.76
185.00	5.226	5.515	10.741	1020.2	9.247	966.84
190.00	5.375	5.614	10.989	1066.7	9.359	1021.2
195.00	5.522	5.712	11.233	1113.8	9.466	1076.7
200.00	5.667	5.807	11.474	1161.4	9.570	1133.5
205.00	5.812	5.900	11.712	1209.5	9.671	1191.5
210.00	5.955	5.991	11.946	1258.1	9.767	1250.6
215.00	6.097	6.080	12.177	1307.1	9.858	1310.9
220.00	6.238	6.167	12.405	1356.7	9.946	1372.4
225.00	6.378	6.252	12.629	1406.6	10.028	1435.0
230.00	6.516	6.334	12.850	1456.9	10.106	1498.7
235.00	6.653	6.416	13.069	1507.6	10.180	1563.5
240.00	6.789	6.495	13.284	1558.7	10.251	1629.3
245.00	6.924	6.572	13.496	1610.2	10.319	1696.3
250.00	7.057	6.648	13.705	1661.9	10.386	1764.3
255.00	7.190	6.722	13.911	1714.0	10.450	1833.3
260.00	7.321	6.794	14.115	1766.4	10.513	1903.4
265.00	7.451	6.865	14.316	1819.1	10.575	1974.5
270.00	7.580	6.934	14.514	1872.2	10.634	2046.6
273.15	7.660	6.977	14.637	1905.7	10.671	2092.5
275.00	7.708	7.002	14.709	1925.5	10.692	2119.6
280.00	7.834	7.068	14.903	1979.1	10.749	2193.6
285.00	7.960	7.133	15.093	2033.0	10.805	2268.6
290.00	8.085	7.197	15.282	2087.1	10.861	2344.6
295.00	8.208	7.260	15.468	2141.6	10.918	2421.4
298.15	8.286	7.298	15.584	2176.0	10.954	2470.4
300.00	8.331	7.321	15.652	2196.3	10.976	2499.2

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-73

THERMODYNAMIC FUNCTIONS FOR LEAD DIOXIDE (PB O_2)
SOLID PHASE

GRAM MOLECULAR WT.=239.1888 GRAMS 1 CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG-MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG-MOLE	$(S_T^0-S_0^0)$ CAL/DEG-MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG-MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.001	0.002	0.007	0.004	0.005
10.00	0.004	0.012	0.017	0.124	0.062	0.042
15.00	0.017	0.060	0.077	0.902	0.270	0.250
20.00	0.045	0.148	0.193	2.967	0.578	0.903
25.00	0.091	0.277	0.368	6.923	1.024	2.282
30.00	0.156	0.444	0.600	13.324	1.541	4.681
35.00	0.239	0.639	0.878	22.359	2.074	8.359
40.00	0.338	0.851	1.189	34.050	2.601	13.514
45.00	0.451	1.074	1.525	48.340	3.113	20.291
50.00	0.576	1.303	1.879	65.151	3.609	28.795
55.00	0.711	1.535	2.246	84.404	4.089	39.101
60.00	0.854	1.767	2.621	106.01	4.552	51.265
65.00	1.005	1.999	3.004	129.90	5.002	65.325
70.00	1.162	2.229	3.390	156.03	5.442	81.309
75.00	1.323	2.456	3.779	184.19	5.803	99.233
80.00	1.489	2.673	4.162	213.85	6.054	119.09
85.00	1.657	2.881	4.538	244.90	6.399	140.84
90.00	1.828	3.090	4.917	278.09	6.875	164.48
95.00	2.000	3.300	5.300	313.46	7.250	190.02
100.00	2.175	3.505	5.679	350.47	7.557	217.47
105.00	2.351	3.706	6.056	389.09	7.894	246.81
110.00	2.528	3.904	6.431	429.41	8.234	278.03
115.00	2.705	4.099	6.804	471.37	8.545	311.12
120.00	2.884	4.290	7.174	514.83	8.839	346.06
125.00	3.063	4.478	7.541	559.75	9.125	382.85
130.00	3.242	4.662	7.904	606.06	9.396	421.47
135.00	3.421	4.842	8.264	653.70	9.658	461.89
140.00	3.601	5.019	8.619	702.62	9.912	504.09
145.00	3.780	5.192	8.972	752.81	10.159	548.07
150.00	3.959	5.361	9.320	804.21	10.402	593.80
155.00	4.137	5.528	9.665	856.82	10.641	641.27
160.00	4.315	5.691	10.007	910.62	10.878	690.45
165.00	4.493	5.852	10.345	965.60	11.115	741.33
170.00	4.670	6.010	10.680	1021.8	11.354	793.90
175.00	4.846	6.167	11.013	1079.1	11.594	848.13
180.00	5.022	6.321	11.343	1137.7	11.834	904.02
185.00	5.198	6.473	11.670	1197.5	12.070	961.56
190.00	5.372	6.623	11.995	1258.4	12.298	1020.7
195.00	5.546	6.771	12.318	1320.4	12.512	1081.5
200.00	5.719	6.917	12.637	1383.5	12.707	1143.9
205.00	5.892	7.061	12.953	1447.5	12.882	1207.9
210.00	6.064	7.201	13.265	1512.3	13.038	1273.4
215.00	6.235	7.339	13.574	1577.8	13.180	1340.5
220.00	6.405	7.473	13.878	1644.1	13.314	1409.1
225.00	6.575	7.604	14.179	1711.0	13.448	1479.3
230.00	6.743	7.733	14.476	1778.5	13.586	1550.9
235.00	6.911	7.859	14.770	1846.8	13.733	1624.0
240.00	7.078	7.983	15.060	1915.9	13.887	1698.6
245.00	7.243	8.105	15.348	1985.7	14.047	1774.6
250.00	7.408	8.225	15.634	2056.4	14.211	1852.1
255.00	7.572	8.344	15.917	2127.8	14.374	1931.0
260.00	7.736	8.462	16.198	2200.1	14.536	2011.3
265.00	7.898	8.578	16.476	2273.2	14.694	2092.9
270.00	8.059	8.693	16.752	2347.0	14.846	2176.0
273.15	8.161	8.764	16.925	2393.9	14.938	2229.1
275.00	8.220	8.806	17.026	2421.6	14.990	2260.5
280.00	8.380	8.918	17.297	2496.9	15.121	2346.3
285.00	8.538	9.027	17.566	2572.8	15.235	2433.4
290.00	8.696	9.135	17.832	2649.2	15.325	2521.9
295.00	8.853	9.241	18.094	2726.0	15.385	2611.7
298.15	8.952	9.306	18.258	2774.5	15.405	2669.0
300.00	9.010	9.343	18.353	2803.0	15.409	2702.9

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-74

THERMODYNAMIC FUNCTIONS FOR LEAD SESQUIOXIDE (PB_2O_3)
SOLID PHASE

GRAM MOLECULAR WT.=462.3782 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.012	0.018	0.029	0.089	0.058	0.059
10.00	0.052	0.152	0.204	1.523	0.701	0.521
15.00	0.185	0.569	0.754	8.538	2.076	2.771
20.00	0.418	1.072	1.490	21.446	3.049	8.352
25.00	0.709	1.555	2.264	38.882	3.914	17.730
30.00	1.034	2.016	3.050	60.482	4.723	31.014
35.00	1.378	2.461	3.840	86.151	5.551	48.235
40.00	1.736	2.901	4.637	116.06	6.414	69.423
45.00	2.103	3.341	5.443	150.33	7.302	94.619
50.00	2.478	3.784	6.261	189.20	8.256	123.88
55.00	2.859	4.232	7.091	232.75	9.125	157.25
60.00	3.246	4.667	7.914	280.05	9.778	194.77
65.00	3.636	5.086	8.722	330.56	10.432	236.37
70.00	4.028	5.490	9.518	384.32	11.062	281.97
75.00	4.420	5.882	10.302	441.12	11.658	331.53
80.00	4.812	6.261	11.073	500.90	12.253	384.97
85.00	5.203	6.631	11.833	563.60	12.818	442.24
90.00	5.592	6.990	12.582	629.06	13.368	503.29
95.00	5.979	7.340	13.319	697.27	13.914	568.04
100.00	6.365	7.682	14.046	768.16	14.439	636.46
105.00	6.748	8.016	14.763	841.63	14.945	708.49
110.00	7.128	8.342	15.470	917.58	15.434	784.07
115.00	7.506	8.660	16.166	995.95	15.911	863.17
120.00	7.881	8.972	16.853	1076.7	16.373	945.72
125.00	8.253	9.277	17.531	1159.7	16.827	1031.7
130.00	8.623	9.576	18.199	1244.9	17.268	1121.0
135.00	8.990	9.869	18.859	1332.3	17.695	1213.7
140.00	9.354	10.156	19.510	1421.8	18.109	1309.6
145.00	9.716	10.437	20.153	1513.4	18.508	1408.8
150.00	10.074	10.713	20.787	1606.9	18.891	1511.1
155.00	10.430	10.982	21.412	1702.3	19.259	1616.6
160.00	10.783	11.247	22.029	1799.5	19.611	1725.2
165.00	11.133	11.505	22.638	1898.4	19.948	1836.9
170.00	11.480	11.758	23.238	1998.9	20.271	1951.6
175.00	11.824	12.006	23.830	2101.1	20.583	2069.3
180.00	12.166	12.248	24.414	2204.7	20.883	2189.9
185.00	12.505	12.486	24.991	2309.9	21.175	2313.4
190.00	12.841	12.718	25.559	2416.5	21.457	2439.8
195.00	13.174	12.946	26.120	2524.4	21.731	2569.0
200.00	13.505	13.169	26.673	2633.8	21.996	2700.9
205.00	13.833	13.387	27.220	2744.4	22.252	2835.7
210.00	14.158	13.601	27.759	2856.3	22.500	2973.1
215.00	14.480	13.811	28.291	2969.4	22.738	3113.3
220.00	14.800	14.016	28.817	3083.6	22.967	3256.0
225.00	15.117	14.218	29.335	3199.0	23.189	3401.4
230.00	15.432	14.415	29.847	3315.5	23.403	3549.4
235.00	15.744	14.609	30.353	3433.0	23.611	3699.9
240.00	16.054	14.798	30.852	3551.6	23.813	3852.9
245.00	16.361	14.984	31.345	3671.2	24.011	4008.4
250.00	16.665	15.167	31.832	3791.7	24.203	4166.3
255.00	16.967	15.346	32.313	3913.2	24.389	4326.7
260.00	17.267	15.521	32.789	4035.6	24.567	4489.5
265.00	17.564	15.694	33.258	4158.8	24.737	4654.6
270.00	17.859	15.863	33.722	4282.9	24.898	4822.0
273.15	18.044	15.967	34.011	4361.5	24.996	4928.7
275.00	18.152	16.028	34.180	4407.8	25.052	4991.8
280.00	18.442	16.191	34.633	4533.4	25.200	5163.8
285.00	18.730	16.350	35.080	4659.8	25.345	5338.1
290.00	19.016	16.506	35.522	4786.9	25.490	5514.6
295.00	19.299	16.660	35.959	4914.7	25.639	5693.3
298.15	19.477	16.755	36.232	4995.6	25.735	5807.0
300.00	19.581	16.811	36.392	5043.3	25.793	5874.2

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-75

THERMODYNAMIC FUNCTIONS FOR LEAD ORTHOPLUMBATE (PB_3O_4)
SOLID PHASE

GRAM MOLECULAR WT.=685.5676 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T	$-(G^0_T-H^0_0)/T$	$(H^0_T-H^0_0)/T$	$(S^0_T-S^0_0)$	$(H^0_T-H^0_0)$	C^0_P	$-(G^0_T-H^0_0)$
DEG K	CAL/DEG MOLE	CAL/DEG MOLE	CAL/DEG MOLE	CAL/MOLE	CAL/DEG MOLE	CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.014	0.020	0.034	0.102	0.066	0.069
10.00	0.059	0.172	0.232	1.723	0.805	0.594
15.00	0.214	0.683	0.898	10.248	2.617	3.215
20.00	0.502	1.356	1.858	27.112	4.105	10.042
25.00	0.879	2.055	2.934	51.374	5.602	21.982
30.00	1.317	2.767	4.084	83.015	7.041	39.505
35.00	1.797	3.477	5.274	121.69	8.425	62.887
40.00	2.307	4.180	6.487	167.20	9.768	92.282
45.00	2.839	4.873	7.712	219.28	11.055	127.78
50.00	3.388	5.553	8.941	277.63	12.272	169.41
55.00	3.949	6.216	10.165	341.87	13.413	217.18
60.00	4.517	6.861	11.378	411.64	14.481	271.04
65.00	5.091	7.486	12.577	486.56	15.477	330.93
70.00	5.668	8.090	13.758	566.27	16.392	396.78
75.00	6.246	8.672	14.918	650.39	17.250	468.47
80.00	6.824	9.233	16.057	738.67	18.046	545.92
85.00	7.400	9.773	17.173	830.66	18.734	629.01
90.00	7.973	10.287	18.261	925.87	19.339	717.60
95.00	8.543	10.779	19.322	1024.0	19.911	811.57
100.00	9.108	11.251	20.358	1125.1	20.539	910.78
105.00	9.668	11.710	21.378	1229.6	21.289	1015.1
110.00	10.223	12.164	22.387	1338.0	22.075	1124.5
115.00	10.774	12.611	23.384	1450.2	22.791	1239.0
120.00	11.320	13.049	24.368	1565.8	23.458	1358.4
125.00	11.861	13.479	25.340	1684.8	24.128	1482.6
130.00	12.398	13.900	26.298	1807.0	24.749	1611.7
135.00	12.930	14.313	27.244	1932.3	25.342	1745.6
140.00	13.458	14.717	28.175	2060.4	25.901	1884.2
145.00	13.982	15.112	29.093	2191.2	26.422	2027.3
150.00	14.500	15.497	29.998	2324.6	26.911	2175.1
155.00	15.015	15.873	30.888	2460.3	27.374	2327.3
160.00	15.524	16.239	31.764	2598.3	27.822	2483.9
165.00	16.030	16.597	32.627	2738.5	28.263	2644.9
170.00	16.530	16.947	33.477	2880.9	28.706	2810.2
175.00	17.027	17.289	34.315	3025.6	29.152	2979.6
180.00	17.518	17.625	35.143	3172.4	29.595	3153.3
185.00	18.006	17.954	35.960	3321.5	30.026	3331.1
190.00	18.489	18.277	36.766	3472.7	30.436	3512.9
195.00	18.968	18.594	37.562	3625.8	30.817	3698.7
200.00	19.442	18.904	38.346	3780.8	31.166	3888.5
205.00	19.913	19.207	39.120	3937.4	31.487	4082.1
210.00	20.379	19.503	39.882	4095.6	31.786	4279.7
215.00	20.842	19.792	40.633	4255.2	32.068	4480.9
220.00	21.300	20.074	41.374	4416.3	32.340	4686.0
225.00	21.754	20.349	42.104	4578.6	32.604	4894.7
230.00	22.204	20.619	42.823	4742.3	32.859	5107.0
235.00	22.651	20.882	43.532	4907.2	33.105	5322.9
240.00	23.093	21.139	44.232	5073.3	33.341	5542.3
245.00	23.531	21.390	44.922	5240.6	33.566	5765.2
250.00	23.966	21.636	45.602	5409.0	33.782	5991.5
255.00	24.397	21.876	46.273	5578.4	33.990	6221.2
260.00	24.824	22.111	46.935	5748.9	34.194	6454.2
265.00	25.247	22.341	47.588	5920.3	34.396	6690.5
270.00	25.667	22.566	48.233	6092.8	34.597	6930.1
273.15	25.929	22.705	48.635	6202.0	34.724	7082.6
275.00	26.083	22.787	48.870	6266.3	34.799	7172.8
280.00	26.496	23.003	49.498	6440.8	35.001	7418.8
285.00	26.905	23.215	50.120	6616.3	35.204	7667.8
290.00	27.310	23.424	50.734	6792.9	35.409	7919.9
295.00	27.712	23.629	51.341	6970.4	35.614	8175.1
298.15	27.964	23.756	51.720	7082.8	35.744	8337.4
300.00	28.111	23.830	51.941	7149.0	35.821	8433.3

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-76

THERMODYNAMIC FUNCTIONS FOR LEAD METASILICATE ($PB SI O_3$)
SOLID PHASE

GRAM MOLECULAR WT.=283.2742 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T	$-(G_T^0-H_0^0)/T$	$(H_T^0-H_0^0)/T$	$(S_T^0-S_0^0)$	$(H_T^0-H_0^0)$	C_p^0	$-(G_T^0-H_0^0)$
DEG K	CAL/DEG MOLE	CAL/DEG MOLE	CAL/DEG MOLE	CAL/MOLE	CAL/DEG MOLE	CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.002	0.003	0.005	0.016	0.010	0.011
10.00	0.009	0.028	0.037	0.280	0.139	0.094
15.00	0.037	0.132	0.169	1.980	0.578	0.557
20.00	0.098	0.312	0.411	6.245	1.154	1.967
25.00	0.193	0.552	0.745	13.810	1.893	4.819
30.00	0.318	0.842	1.161	25.270	2.694	9.555
35.00	0.472	1.165	1.637	40.768	3.504	16.528
40.00	0.650	1.507	2.157	60.276	4.293	25.997
45.00	0.848	1.858	2.706	83.632	5.042	38.145
50.00	1.062	2.212	3.274	110.62	5.743	53.090
55.00	1.289	2.562	3.851	140.92	6.356	70.902
60.00	1.527	2.901	4.427	174.03	6.883	91.600
65.00	1.772	3.227	4.999	209.75	7.409	115.17
70.00	2.023	3.545	5.567	248.12	7.932	141.58
75.00	2.278	3.854	6.131	289.02	8.422	170.83
80.00	2.536	4.154	6.690	332.32	8.898	202.89
85.00	2.797	4.447	7.243	377.97	9.363	237.72
90.00	3.059	4.732	7.791	425.92	9.813	275.31
95.00	3.322	5.011	8.334	476.08	10.252	315.63
100.00	3.586	5.284	8.871	528.42	10.680	358.64
105.00	3.851	5.551	9.402	582.86	11.095	404.32
110.00	4.115	5.812	9.927	639.35	11.499	452.65
115.00	4.379	6.068	10.447	697.84	11.894	503.59
120.00	4.643	6.319	10.962	758.28	12.280	557.11
125.00	4.906	6.565	11.471	820.63	12.661	613.19
130.00	5.168	6.807	11.974	884.87	13.034	671.81
135.00	5.429	7.044	12.473	950.95	13.399	732.93
140.00	5.690	7.277	12.967	1018.8	13.757	796.53
145.00	5.949	7.507	13.456	1088.5	14.107	862.59
150.00	6.207	7.733	13.940	1159.9	14.446	931.08
155.00	6.464	7.955	14.419	1233.0	14.775	1002.0
160.00	6.720	8.173	14.893	1307.6	15.093	1075.3
165.00	6.975	8.387	15.362	1383.9	15.401	1150.9
170.00	7.229	8.598	15.826	1461.6	15.698	1228.9
175.00	7.481	8.805	16.286	1540.8	15.987	1309.2
180.00	7.732	9.008	16.740	1621.5	16.269	1391.7
185.00	7.981	9.208	17.190	1703.5	16.545	1476.6
190.00	8.230	9.405	17.634	1786.9	16.816	1563.6
195.00	8.476	9.598	18.075	1871.7	17.083	1652.9
200.00	8.722	9.789	18.511	1957.7	17.344	1744.4
205.00	8.966	9.976	18.942	2045.1	17.600	1838.0
210.00	9.208	10.161	19.369	2133.7	17.850	1933.8
215.00	9.450	10.342	19.792	2223.6	18.093	2031.7
220.00	9.689	10.521	20.211	2314.7	18.329	2131.7
225.00	9.928	10.697	20.625	2406.9	18.559	2233.8
230.00	10.165	10.871	21.036	2500.2	18.783	2337.9
235.00	10.401	11.041	21.442	2594.7	19.002	2444.1
240.00	10.635	11.209	21.844	2690.3	19.218	2552.3
245.00	10.868	11.375	22.243	2786.9	19.431	2662.6
250.00	11.099	11.538	22.637	2884.6	19.640	2774.8
255.00	11.329	11.699	23.028	2983.3	19.846	2888.9
260.00	11.558	11.858	23.416	3083.0	20.050	3005.0
265.00	11.785	12.014	23.799	3183.8	20.250	3123.1
270.00	12.011	12.169	24.180	3285.5	20.447	3243.0
273.15	12.153	12.265	24.418	3350.1	20.569	3319.6
275.00	12.236	12.321	24.557	3388.2	20.641	3364.9
280.00	12.459	12.471	24.930	3491.9	20.834	3488.6
285.00	12.681	12.620	25.301	3596.6	21.024	3614.2
290.00	12.902	12.766	25.668	3702.2	21.213	3741.6
295.00	13.121	12.911	26.032	3808.7	21.401	3870.8
298.15	13.259	13.001	26.260	3876.3	21.518	3953.2
300.00	13.340	13.054	26.394	3916.2	21.587	4001.9

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-77

THERMODYNAMIC FUNCTIONS FOR LEAD ORTHOSILICATE ($PB_2SI\ O_4$)
SOLID PHASE

GRAM MOLECULAR WT.=506.4636 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.012	0.018	0.030	0.090	0.059	0.060
10.00	0.053	0.153	0.206	1.532	0.706	0.526
15.00	0.187	0.578	0.765	8.669	2.132	2.799
20.00	0.425	1.111	1.536	22.218	3.280	8.508
25.00	0.732	1.667	2.399	41.675	4.524	18.311
30.00	1.088	2.252	3.340	67.561	5.834	32.631
35.00	1.480	2.857	4.238	100.01	7.141	51.804
40.00	1.902	3.471	5.373	138.86	8.382	76.070
45.00	2.346	4.081	6.427	183.66	9.517	105.57
50.00	2.807	4.676	7.483	233.78	10.507	140.34
55.00	3.279	5.245	8.524	288.48	11.353	180.37
60.00	3.759	5.787	9.546	347.23	12.146	225.55
65.00	4.243	6.306	10.549	409.91	12.916	275.80
70.00	4.729	6.804	11.533	476.31	13.643	331.02
75.00	5.215	7.284	12.499	546.33	14.362	391.10
80.00	5.700	7.748	13.448	619.88	15.051	455.98
85.00	6.183	8.197	14.380	696.79	15.710	525.56
90.00	6.664	8.633	15.297	776.97	16.364	599.76
95.00	7.142	9.057	16.199	860.40	17.008	678.50
100.00	7.617	9.470	17.087	947.02	17.635	761.72
105.00	8.089	9.874	17.963	1036.7	18.242	849.36
110.00	8.558	10.267	18.825	1129.4	18.824	941.33
115.00	9.022	10.652	19.674	1224.9	19.389	1037.6
120.00	9.484	11.027	20.511	1323.3	19.945	1138.0
125.00	9.941	11.395	21.337	1424.4	20.505	1242.7
130.00	10.395	11.756	22.151	1528.3	21.049	1351.4
135.00	10.846	12.110	22.956	1634.9	21.582	1464.2
140.00	11.292	12.458	23.750	1744.1	22.103	1580.9
145.00	11.736	12.799	24.535	1855.9	22.607	1701.7
150.00	12.175	13.134	25.309	1970.1	23.097	1826.3
155.00	12.611	13.463	26.074	2086.8	23.569	1954.7
160.00	13.044	13.786	26.830	2205.8	24.027	2087.0
165.00	13.473	14.103	27.576	2327.1	24.470	2223.0
170.00	13.898	14.415	28.313	2450.5	24.899	2362.7
175.00	14.321	14.720	29.041	2576.0	25.315	2506.1
180.00	14.740	15.020	29.760	2703.6	25.720	2653.1
185.00	15.155	15.315	30.470	2833.2	26.114	2803.7
190.00	15.567	15.604	31.171	2964.7	26.498	2957.8
195.00	15.976	15.888	31.864	3098.2	26.872	3115.4
200.00	16.382	16.167	32.549	3233.4	27.237	3276.5
205.00	16.785	16.442	33.226	3370.5	27.591	3440.9
210.00	17.184	16.711	33.895	3509.3	27.933	3608.7
215.00	17.581	16.976	34.557	3649.8	28.263	3779.8
220.00	17.974	17.236	35.210	3791.9	28.579	3954.3
225.00	18.364	17.492	35.856	3935.6	28.882	4131.9
230.00	18.751	17.742	36.494	4080.7	29.176	4312.8
235.00	19.136	17.989	37.124	4227.3	29.463	4496.8
240.00	19.517	18.231	37.747	4375.4	29.746	4684.0
245.00	19.895	18.469	38.364	4524.8	30.028	4874.3
250.00	20.271	18.703	38.973	4675.6	30.311	5067.7
255.00	20.643	18.933	39.576	4827.9	30.593	5264.0
260.00	21.013	19.160	40.173	4981.6	30.871	5463.4
265.00	21.380	19.383	40.764	5136.6	31.142	5665.7
270.00	21.745	19.604	41.348	5293.0	31.403	5871.0
273.15	21.973	19.741	41.713	5392.1	31.562	6001.8
275.00	22.106	19.820	41.927	5450.6	31.653	6079.2
280.00	22.465	20.034	42.499	5609.5	31.894	6290.3
285.00	22.822	20.244	43.066	5769.5	32.130	6504.2
290.00	23.176	20.451	43.627	5930.8	32.369	6720.9
295.00	23.527	20.655	44.182	6093.2	32.614	6940.5
298.15	23.747	20.782	44.529	6196.2	32.774	7080.2
300.00	23.876	20.857	44.732	6257.0	32.871	7162.7

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-78

THERMODYNAMIC FUNCTIONS FOR ANDALUCITE ($AL_2SI\ O_5$)
SOLID PHASE

GRAM MOLECULAR WT.=162.0460 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.000	0.001	0.001	0.001
10.00	0.001	0.002	0.003	0.024	0.012	0.008
15.00	0.003	0.012	0.016	0.184	0.056	0.050
20.00	0.009	0.031	0.040	0.617	0.123	0.184
25.00	0.019	0.060	0.079	1.501	0.240	0.475
30.00	0.034	0.103	0.137	3.100	0.409	1.006
35.00	0.054	0.162	0.216	5.673	0.629	1.879
40.00	0.080	0.237	0.317	9.475	0.900	3.201
45.00	0.113	0.328	0.441	14.750	1.217	5.086
50.00	0.153	0.434	0.587	21.687	1.560	7.646
55.00	0.200	0.553	0.752	30.396	1.935	10.985
60.00	0.253	0.687	0.940	41.193	2.398	15.206
65.00	0.314	0.838	1.153	54.487	2.928	20.426
70.00	0.382	1.007	1.390	70.506	3.477	26.772
75.00	0.458	1.191	1.649	89.299	4.052	34.359
80.00	0.541	1.389	1.930	111.10	4.670	43.297
85.00	0.632	1.600	2.231	135.96	5.273	53.693
90.00	0.729	1.821	2.550	163.89	5.906	65.639
95.00	0.834	2.054	2.888	195.09	6.576	79.226
100.00	0.945	2.297	3.242	229.65	7.249	94.543
105.00	1.064	2.548	3.612	267.59	7.925	111.67
110.00	1.188	2.808	3.996	308.92	8.609	130.69
115.00	1.319	3.076	4.394	353.69	9.300	151.66
120.00	1.455	3.349	4.805	401.92	9.996	174.65
125.00	1.598	3.629	5.227	453.63	10.685	199.73
130.00	1.746	3.914	5.659	508.78	11.374	226.94
135.00	1.899	4.203	6.101	567.36	12.057	256.33
140.00	2.057	4.495	6.552	629.34	12.734	287.96
145.00	2.220	4.791	7.011	694.69	13.405	321.87
150.00	2.387	5.089	7.476	763.37	14.068	358.08
155.00	2.559	5.389	7.948	835.36	14.725	396.64
160.00	2.735	5.691	8.426	910.61	15.375	437.58
165.00	2.915	5.994	8.909	989.09	16.016	480.91
170.00	3.098	6.299	9.397	1070.8	16.648	526.68
175.00	3.285	6.603	9.888	1155.6	17.271	574.89
180.00	3.475	6.908	10.383	1243.4	17.884	625.56
185.00	3.669	7.213	10.882	1334.4	18.485	678.73
190.00	3.865	7.517	11.382	1428.3	19.076	734.38
195.00	4.064	7.821	11.886	1525.1	19.656	792.55
200.00	4.266	8.124	12.390	1624.8	20.224	853.24
205.00	4.471	8.426	12.897	1727.3	20.780	916.46
210.00	4.677	8.727	13.404	1832.6	21.323	982.21
215.00	4.886	9.026	13.912	1940.5	21.854	1050.5
220.00	5.097	9.323	14.420	2051.1	22.372	1121.3
225.00	5.310	9.619	14.929	2164.3	22.880	1194.7
230.00	5.524	9.913	15.437	2279.9	23.378	1270.6
235.00	5.741	10.204	15.945	2398.0	23.869	1349.1
240.00	5.959	10.494	16.453	2518.6	24.353	1430.1
245.00	6.178	10.782	16.960	2641.5	24.830	1513.6
250.00	6.399	11.067	17.466	2766.9	25.299	1599.7
255.00	6.621	11.351	17.972	2894.5	25.759	1688.3
260.00	6.844	11.632	18.476	3024.4	26.210	1779.4
265.00	7.068	11.912	18.980	3156.6	26.650	1873.0
270.00	7.293	12.189	19.482	3290.9	27.079	1969.2
273.15	7.436	12.362	19.797	3376.6	27.345	2031.0
275.00	7.519	12.463	19.983	3427.4	27.499	2067.8
280.00	7.746	12.735	20.482	3565.9	27.910	2169.0
285.00	7.974	13.005	20.979	3706.5	28.312	2272.6
290.00	8.203	13.272	21.475	3849.0	28.706	2378.8
295.00	8.432	13.537	21.969	3993.5	29.093	2487.4
298.15	8.577	13.703	22.279	4085.5	29.334	2557.1
300.00	8.662	13.800	22.461	4139.9	29.474	2598.5

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K.

TABLE B-79

THERMODYNAMIC FUNCTIONS FOR KYANITE $(AL_2SI\ O_5)$
SOLID PHASE

GRAM MOLECULAR WT.=162.0460 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL DEG-MOLE	$(H_T^0-H_0^0)/T$ CAL DEG-MOLE	$(S_T^0-S_0^0)$ CAL DEG-MOLE	$(H_T^0-H_0^0)$ CAL MOLE	C_P^0 CAL DEG-MOLE	$-(G_T^0-H_0^0)$ CAL MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.000	0.001	0.000	0.001
10.00	0.000	0.001	0.002	0.012	0.006	0.004
15.00	0.002	0.006	0.008	0.090	0.027	0.024
20.00	0.004	0.015	0.020	0.301	0.060	0.090
25.00	0.009	0.029	0.039	0.734	0.118	0.232
30.00	0.016	0.051	0.067	1.523	0.203	0.492
35.00	0.026	0.080	0.107	2.816	0.320	0.922
40.00	0.040	0.120	0.159	4.780	0.472	1.581
45.00	0.056	0.169	0.225	7.598	0.661	2.535
50.00	0.077	0.228	0.306	11.424	0.871	3.857
55.00	0.102	0.297	0.399	16.345	1.108	5.613
60.00	0.131	0.378	0.509	22.665	1.436	7.876
65.00	0.165	0.474	0.639	30.808	1.828	10.738
70.00	0.204	0.586	0.790	41.013	2.262	14.302
75.00	0.249	0.714	0.963	53.513	2.745	18.675
80.00	0.300	0.857	1.156	68.532	3.267	23.963
85.00	0.356	1.014	1.371	86.228	3.816	30.271
90.00	0.419	1.186	1.605	106.75	4.399	37.702
95.00	0.488	1.371	1.859	130.28	5.017	46.355
100.00	0.563	1.570	2.133	156.96	5.661	56.328
105.00	0.645	1.780	2.425	186.92	6.327	67.715
110.00	0.733	2.002	2.735	220.26	7.008	80.609
115.00	0.827	2.235	3.062	257.03	7.703	95.094
120.00	0.927	2.478	3.405	297.31	8.412	111.25
125.00	1.033	2.729	3.763	341.15	9.126	129.17
130.00	1.145	2.989	4.134	388.58	9.846	148.90
135.00	1.263	3.256	4.520	439.61	10.567	170.53
140.00	1.387	3.530	4.917	494.24	11.286	194.12
145.00	1.515	3.810	5.325	552.47	12.004	219.72
150.00	1.649	4.095	5.744	614.28	12.717	247.39
155.00	1.788	4.385	6.173	679.63	13.424	277.18
160.00	1.932	4.678	6.610	748.51	14.125	309.14
165.00	2.081	4.975	7.056	820.87	14.817	343.30
170.00	2.234	5.274	7.508	896.66	15.499	379.70
175.00	2.391	5.576	7.967	975.84	16.170	418.39
180.00	2.552	5.880	8.432	1058.3	16.829	459.38
185.00	2.717	6.184	8.902	1144.1	17.477	502.72
190.00	2.886	6.490	9.376	1233.1	18.113	548.41
195.00	3.059	6.796	9.855	1325.2	18.738	596.49
200.00	3.235	7.102	10.337	1420.5	19.353	646.96
205.00	3.414	7.408	10.822	1518.7	19.957	699.86
210.00	3.596	7.714	11.310	1620.0	20.549	755.19
215.00	3.781	8.020	11.801	1724.2	21.128	812.97
220.00	3.969	8.324	12.293	1831.3	21.695	873.20
225.00	4.160	8.627	12.787	1941.1	22.250	935.90
230.00	4.352	8.929	13.282	2053.7	22.794	1001.1
235.00	4.548	9.230	13.778	2169.1	23.329	1068.7
240.00	4.745	9.529	14.274	2287.0	23.856	1138.9
245.00	4.945	9.827	14.772	2407.6	24.373	1211.5
250.00	5.146	10.123	15.269	2530.7	24.879	1286.6
255.00	5.350	10.417	15.767	2656.4	25.372	1364.2
260.00	5.555	10.709	16.264	2784.4	25.850	1444.2
265.00	5.762	10.999	16.761	2914.8	26.313	1526.8
270.00	5.970	11.287	17.257	3047.5	26.761	1611.8
273.15	6.102	11.467	17.569	3132.3	27.036	1666.7
275.00	6.180	11.572	17.752	3182.4	27.195	1699.4
280.00	6.391	11.855	18.246	3319.5	27.619	1789.4
285.00	6.603	12.135	18.738	3458.6	28.034	1881.8
290.00	6.816	12.413	19.229	3599.8	28.441	1976.7
295.00	7.031	12.688	19.719	3743.0	28.841	2074.1
298.15	7.167	12.860	20.027	3834.2	29.089	2136.7
300.00	7.246	12.961	20.207	3888.2	29.232	2173.9

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-80

THERMODYNAMIC FUNCTIONS FOR SILLIMANITE ($AL_2SI\ O_5$)
SOLID PHASE

GRAM MOLECULAR WT.=162.0460 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.001	0.002	0.001	0.001
10.00	0.001	0.003	0.004	0.030	0.015	0.010
15.00	0.004	0.015	0.019	0.222	0.067	0.061
20.00	0.011	0.037	0.048	0.745	0.149	0.223
25.00	0.023	0.072	0.095	1.812	0.288	0.574
30.00	0.040	0.124	0.165	3.730	0.488	1.214
35.00	0.065	0.194	0.259	6.789	0.745	2.262
40.00	0.096	0.282	0.378	11.260	1.052	3.842
45.00	0.135	0.386	0.522	17.388	1.406	6.080
50.00	0.182	0.508	0.690	25.387	1.799	9.098
55.00	0.237	0.645	0.881	35.455	2.238	13.015
60.00	0.299	0.798	1.097	47.873	2.739	17.951
65.00	0.370	0.968	1.337	62.907	3.280	24.027
70.00	0.448	1.153	1.601	80.734	3.856	31.365
75.00	0.534	1.354	1.888	101.52	4.461	40.079
80.00	0.628	1.567	2.195	125.36	5.077	50.279
85.00	0.730	1.792	2.522	152.32	5.711	62.065
90.00	0.839	2.028	2.867	182.50	6.365	75.531
95.00	0.955	2.274	3.229	215.98	7.030	90.764
100.00	1.078	2.528	3.607	252.83	7.711	107.85
105.00	1.208	2.792	4.000	293.11	8.400	126.86
110.00	1.344	3.062	4.406	336.83	9.088	147.87
115.00	1.486	3.339	4.826	383.99	9.775	170.94
120.00	1.635	3.621	5.256	434.58	10.458	196.14
125.00	1.788	3.909	5.697	488.59	11.145	223.52
130.00	1.947	4.200	6.147	546.02	11.827	253.13
135.00	2.111	4.495	6.606	606.85	12.504	285.01
140.00	2.280	4.793	7.073	671.05	13.176	319.20
145.00	2.453	5.094	7.547	738.59	13.840	355.75
150.00	2.631	5.396	8.027	809.44	14.498	394.68
155.00	2.813	5.700	8.513	883.55	15.146	436.03
160.00	2.999	6.006	9.004	960.89	15.785	479.83
165.00	3.188	6.311	9.500	1041.4	16.413	526.09
170.00	3.381	6.618	9.999	1125.0	17.030	574.83
175.00	3.578	6.924	10.501	1211.7	17.634	626.08
180.00	3.777	7.230	11.007	1301.3	18.228	679.85
185.00	3.979	7.535	11.514	1393.9	18.810	736.15
190.00	4.184	7.839	12.023	1489.4	19.383	794.99
195.00	4.392	8.142	12.534	1587.7	19.946	856.38
200.00	4.602	8.444	13.046	1688.9	20.500	920.33
205.00	4.814	8.745	13.559	1792.7	21.042	986.84
210.00	5.028	9.044	14.072	1899.3	21.573	1055.9
215.00	5.245	9.341	14.586	2008.4	22.090	1127.6
220.00	5.463	9.637	15.100	2120.1	22.594	1201.8
225.00	5.683	9.930	15.613	2234.3	23.085	1278.6
230.00	5.904	10.222	16.126	2351.0	23.566	1357.9
235.00	6.127	10.511	16.637	2470.0	24.038	1439.8
240.00	6.351	10.797	17.148	2591.3	24.504	1524.3
245.00	6.577	11.082	17.658	2715.0	24.964	1611.3
250.00	6.803	11.364	18.167	2841.0	25.417	1700.9
255.00	7.031	11.644	18.675	2969.2	25.862	1793.0
260.00	7.260	11.921	19.182	3099.6	26.297	1887.6
265.00	7.490	12.197	19.686	3232.1	26.722	1984.8
270.00	7.720	12.470	20.190	3366.8	27.134	2084.5
273.15	7.866	12.640	20.506	3452.7	27.389	2148.6
275.00	7.952	12.740	20.691	3503.5	27.536	2186.7
280.00	8.184	13.008	21.191	3642.1	27.929	2291.4
285.00	8.416	13.273	21.689	3782.7	28.314	2398.6
290.00	8.649	13.535	22.185	3925.3	28.694	2508.3
295.00	8.883	13.795	22.678	4069.7	29.068	2620.4
298.15	9.030	13.958	22.988	4161.6	29.300	2692.4
300.00	9.117	14.053	23.170	4215.9	29.435	2735.1

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-81

THERMODYNAMIC FUNCTIONS FOR BERYLLIUM ORTHOSILICATE ($BE_2SI\ O_4$)
SOLID PHASE

GRAM MOLECULAR WT.=110.108 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T	$-(G_T^0-H_0^0)/T$	$(H_T^0-H_0^0)/T$	$(S_T^0-S_0^0)$	$(H_T^0-H_0^0)$	C_P^0	$-(G_T^0-H_0^0)$
DEG K	CAL / DEG MOLE	CAL / DEG MOLE	CAL / DEG MOLE 1	CAL / MOLE	CAL / DEG MOLE	CAL / MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.000	0.001	0.000	0.000
10.00	0.000	0.001	0.001	0.010	0.005	0.003
15.00	0.001	0.005	0.006	0.073	0.022	0.020
20.00	0.004	0.012	0.016	0.247	0.049	0.074
25.00	0.008	0.024	0.032	0.602	0.096	0.190
30.00	0.013	0.042	0.055	1.250	0.167	0.403
35.00	0.022	0.066	0.088	2.314	0.264	0.756
40.00	0.032	0.099	0.131	3.941	0.392	1.298
45.00	0.046	0.140	0.186	6.297	0.555	2.086
50.00	0.064	0.191	0.254	9.532	0.741	3.183
55.00	0.085	0.250	0.334	13.748	0.955	4.649
60.00	0.109	0.320	0.429	19.213	1.242	6.552
65.00	0.138	0.404	0.542	26.249	1.579	8.973
70.00	0.171	0.501	0.673	35.077	1.956	12.001
75.00	0.210	0.611	0.821	45.833	2.349	15.728
80.00	0.253	0.732	0.985	58.593	2.755	20.236
85.00	0.301	0.863	1.165	73.386	3.163	25.606
90.00	0.354	1.003	1.357	90.256	3.590	31.905
95.00	0.413	1.151	1.563	109.32	4.039	39.201
100.00	0.476	1.307	1.782	130.66	4.494	47.560
105.00	0.543	1.469	2.013	154.28	4.960	57.043
110.00	0.616	1.639	2.254	180.29	5.444	67.706
115.00	0.692	1.815	2.507	208.74	5.939	79.606
120.00	0.773	1.997	2.771	239.69	6.442	92.797
125.00	0.859	2.185	3.044	273.14	6.940	107.33
130.00	0.948	2.378	3.326	309.10	7.445	123.25
135.00	1.041	2.575	3.616	347.59	7.951	140.60
140.00	1.139	2.776	3.915	388.61	8.458	159.42
145.00	1.240	2.980	4.220	432.17	8.967	179.76
150.00	1.344	3.188	4.533	478.27	9.474	201.64
155.00	1.452	3.399	4.852	526.91	9.980	225.10
160.00	1.564	3.613	5.176	578.07	10.483	250.16
165.00	1.678	3.829	5.507	631.73	10.983	276.87
170.00	1.796	4.046	5.842	687.90	11.482	305.24
175.00	1.916	4.266	6.182	746.55	11.979	335.30
180.00	2.039	4.487	6.526	807.69	12.475	367.07
185.00	2.165	4.710	6.875	871.30	12.970	400.57
190.00	2.294	4.934	7.227	937.38	13.463	435.82
195.00	2.425	5.159	7.583	1005.9	13.954	472.85
200.00	2.558	5.385	7.943	1076.9	14.441	511.66
205.00	2.694	5.611	8.305	1150.3	14.923	552.28
210.00	2.832	5.839	8.671	1226.1	15.401	594.72
215.00	2.972	6.067	9.039	1304.3	15.873	638.99
220.00	3.114	6.295	9.409	1384.9	16.339	685.11
225.00	3.258	6.523	9.781	1467.7	16.797	733.09
230.00	3.404	6.751	10.155	1552.8	17.247	782.93
235.00	3.552	6.979	10.531	1640.2	17.689	834.64
240.00	3.701	7.207	10.908	1729.7	18.123	888.24
245.00	3.852	7.434	11.286	1821.4	18.549	943.73
250.00	4.004	7.661	11.665	1915.2	18.969	1001.1
255.00	4.158	7.887	12.045	2011.1	19.384	1060.4
260.00	4.314	8.112	12.425	2109.0	19.795	1121.6
265.00	4.470	8.336	12.806	2209.0	20.202	1184.6
270.00	4.628	8.559	13.188	2311.0	20.604	1249.6
273.15	4.728	8.700	13.428	2376.3	20.854	1291.5
275.00	4.787	8.782	13.569	2415.0	21.001	1316.5
280.00	4.948	9.004	13.951	2521.0	21.393	1385.3
285.00	5.109	9.224	14.333	2629.0	21.782	1456.0
290.00	5.271	9.444	14.715	2738.8	22.168	1528.6
295.00	5.434	9.663	15.098	2850.6	22.552	1603.2
298.15	5.538	9.801	15.338	2922.1	22.794	1651.1
300.00	5.599	9.881	15.480	2964.3	22.935	1679.6

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-82

THERMODYNAMIC FUNCTIONS FOR ALUMINUM TITANATE ($AL_2TI\ O_5$)
SOLID PHASE

GRAM MOLECULAR WT.=181.8600 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S^0_T-S^0_0)$ CAL/DEG MOLE 1	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.001	0.002	0.001	0.001
10.00	0.001	0.004	0.005	0.035	0.018	0.012
15.00	0.005	0.018	0.022	0.263	0.080	0.072
20.00	0.013	0.044	0.057	0.882	0.176	0.264
25.00	0.027	0.086	0.113	2.141	0.340	0.679
30.00	0.048	0.146	0.194	4.392	0.571	1.435
35.00	0.076	0.227	0.303	7.944	0.859	2.667
40.00	0.113	0.327	0.440	13.070	1.199	4.513
45.00	0.158	0.445	0.603	20.009	1.582	7.107
50.00	0.212	0.579	0.790	28.934	1.992	10.580
55.00	0.274	0.728	1.001	40.024	2.462	15.048
60.00	0.344	0.896	1.240	53.740	3.041	20.638
65.00	0.423	1.085	1.508	70.549	3.690	27.496
70.00	0.511	1.295	1.806	90.678	4.363	35.771
75.00	0.608	1.523	2.131	114.21	5.053	45.604
80.00	0.714	1.766	2.480	141.25	5.769	57.120
85.00	0.829	2.023	2.852	171.96	6.521	70.438
90.00	0.952	2.294	3.246	206.48	7.289	85.674
95.00	1.084	2.577	3.661	244.85	8.060	102.93
100.00	1.223	2.871	4.094	287.09	8.837	122.31
105.00	1.371	3.174	4.544	333.25	9.628	143.90
110.00	1.525	3.485	5.011	383.40	10.436	167.78
115.00	1.687	3.805	5.493	437.62	11.250	194.04
120.00	1.856	4.132	5.988	495.89	12.054	222.73
125.00	2.032	4.465	6.497	558.14	12.847	253.94
130.00	2.213	4.803	7.016	624.35	13.635	287.72
135.00	2.401	5.144	7.545	694.47	14.413	324.12
140.00	2.594	5.489	8.083	768.47	15.183	363.18
145.00	2.793	5.836	8.629	846.29	15.943	404.96
150.00	2.997	6.186	9.182	927.88	16.692	449.49
155.00	3.205	6.537	9.742	1013.2	17.430	496.80
160.00	3.418	6.889	10.307	1102.2	18.156	546.92
165.00	3.636	7.241	10.876	1194.7	18.868	599.87
170.00	3.857	7.593	11.450	1290.8	19.566	655.69
175.00	4.082	7.945	12.027	1390.4	20.248	714.38
180.00	4.311	8.296	12.607	1493.3	20.913	775.96
185.00	4.543	8.646	13.189	1599.5	21.562	840.45
190.00	4.778	8.994	13.772	1708.9	22.195	907.85
195.00	5.016	9.340	14.357	1821.4	22.811	978.17
200.00	5.257	9.685	14.942	1937.0	23.414	1051.4
205.00	5.500	10.027	15.527	2055.5	24.003	1127.6
210.00	5.746	10.366	16.113	2177.0	24.580	1206.7
215.00	5.994	10.704	16.698	2301.3	25.144	1288.7
220.00	6.244	11.038	17.282	2428.4	25.695	1373.7
225.00	6.496	11.370	17.866	2558.2	26.231	1461.5
230.00	6.749	11.699	18.448	2690.7	26.752	1552.3
235.00	7.004	12.024	19.029	2825.7	27.258	1646.0
240.00	7.261	12.347	19.608	2963.2	27.749	1742.6
245.00	7.519	12.666	20.185	3103.2	28.226	1842.1
250.00	7.778	12.982	20.760	3245.5	28.693	1944.4
255.00	8.038	13.294	21.332	3390.1	29.149	2049.7
260.00	8.299	13.604	21.903	3536.9	29.595	2157.8
265.00	8.561	13.909	22.471	3686.0	30.030	2268.7
270.00	8.824	14.212	23.036	3837.2	30.453	2382.5
273.15	8.990	14.401	23.391	3933.6	30.714	2455.6
275.00	9.087	14.511	23.598	3990.5	30.864	2499.1
280.00	9.352	14.807	24.158	4145.8	31.264	2618.4
285.00	9.616	15.099	24.715	4303.1	31.654	2740.6
290.00	9.881	15.387	25.269	4462.4	32.039	2865.6
295.00	10.147	15.673	25.820	4623.5	32.421	2993.3
298.15	10.314	15.851	26.165	4726.0	32.663	3075.2
300.00	10.413	15.955	26.368	4786.6	32.805	3123.8

H^0_0 AND S^0_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-82(CONT.)

THERMODYNAMIC FUNCTIONS FOR ALUMINUM TITANATE $(AL_2TI\ O_5)$
SOLID PHASE

GRAM MOLECULAR WT.=181.8600 GRAMS 1 CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T^0-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
300.00	10.413	15.955	26.368	4786.6	32.805	3123.8
310.00	10.945	16.511	27.456	5118.5	33.575	3392.9
320.00	11.478	17.056	28.534	5458.1	34.336	3672.9
330.00	12.011	17.591	29.602	5805.1	35.060	3963.6
340.00	12.544	18.115	30.659	6159.1	35.727	4264.9
350.00	13.076	18.627	31.703	6519.4	36.336	4576.7
360.00	13.608	19.127	32.735	6885.6	36.892	4898.9
370.00	14.139	19.614	33.753	7257.1	37.405	5231.3
373.15	14.306	19.765	34.070	7375.2	37.559	5338.2
380.00	14.668	20.088	34.757	7633.6	37.882	5573.9
390.00	15.196	20.550	35.746	8014.7	38.327	5926.4
400.00	15.722	21.000	36.722	8400.0	38.744	6288.8
425.00	17.028	22.072	39.100	9380.6	39.676	7236.7
450.00	18.318	23.073	41.391	10383.	40.479	8243.0
475.00	19.591	24.008	43.598	11404.	41.179	9305.6
500.00	20.845	24.882	45.727	12441.	41.795	10422.
550.00	23.292	26.469	49.761	14558.	42.838	12811.
600.00	25.656	27.870	53.526	16722.	43.696	15394.
650.00	27.937	29.116	57.053	18925.	44.421	18159.
700.00	30.137	30.232	60.368	21162.	45.052	21096.
750.00	32.257	31.238	63.496	23429.	45.612	24193.
800.00	34.303	32.153	66.456	25722.	46.118	27442.
850.00	36.278	32.988	69.266	28040.	46.583	30836.
900.00	38.185	33.756	71.941	30380.	47.016	34367.
950.00	40.030	34.464	74.494	32741.	47.423	38028.
1000.00	41.814	35.122	76.936	35122.	47.809	41814.
1050.00	43.543	35.735	79.278	37522.	48.178	45720.
1100.00	45.219	36.309	81.527	39940.	48.533	49741.
1150.00	46.845	36.848	83.692	42375.	48.877	53871.
1200.00	48.424	37.356	85.780	44827.	49.211	58108.
1250.00	49.959	37.837	87.795	47296.	49.538	62448.
1300.00	51.451	38.293	89.744	49781.	49.857	66887.
1350.00	52.905	38.727	91.632	52282.	50.170	71422.
1400.00	54.321	39.141	93.462	54798.	50.478	76049.
1450.00	55.701	39.537	95.239	57329.	50.782	80767.
1500.00	57.048	39.917	96.965	59876.	51.082	85572.
1550.00	58.363	40.282	98.645	62437.	51.378	90463.
1600.00	59.647	40.634	100.28	65014.	51.672	95436.
1650.00	60.903	40.972	101.88	67605.	51.963	100490.
1700.00	62.131	41.300	103.43	70210.	52.252	105623.
1750.00	63.333	41.617	104.95	72830.	52.539	110832.
1800.00	64.510	41.924	106.43	75464.	52.824	116117.
1850.00	65.662	42.223	107.89	78112.	53.107	121475.
1900.00	66.792	42.513	109.31	80775.	53.389	126905.
1950.00	67.900	42.795	110.70	83451.	53.670	132405.
2000.00	68.987	43.071	112.06	86142.	53.950	137974.

H_0^0 AND S_0^0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

TABLE B-83

THERMODYNAMIC FUNCTIONS FOR BERYLLIUM ALUMINATE ($BeO \cdot Al_2O_3$)

SOLID PHASE

GRAM MOLECULAR WEIGHT = 126.97 GRAMS

1 CAL = 4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$[-(G^o_T-H^o_{298})/T]-S^o_{298}$ CAL/DEG MOLE	$(H^o_T-H^o_{298})/T$ CAL/DEG MOLE	$(S^o_T-S^o_{298})$ CAL/DEG MOLE	$(H^o_T-H^o_{298})$ CAL/MOLE	C^o_P CAL/DEG MOLE	$[-(G^o_T-H^o_{298})-TS^o_{298}]$ CAL/MOLE
298.15	0.000	0.000	0.000	0.000	24.497	0.000
300.00	0.000	0.152	0.152	45.491	24.679	0.138
310.00	0.019	0.958	0.977	297.02	25.612	5.780
320.00	0.062	1.742	1.804	557.45	26.462	19.681
330.00	0.127	2.503	2.630	826.02	27.240	41.849
340.00	0.213	3.241	3.454	1102.0	27.956	72.271
350.00	0.317	3.957	4.274	1384.9	28.615	110.91
360.00	0.438	4.651	5.089	1674.2	29.226	157.73
370.00	0.575	5.322	5.897	1969.3	29.793	212.67
373.15	0.621	5.530	6.151	2063.4	29.963	231.64
380.00	0.725	5.973	6.699	2269.9	30.321	275.65
390.00	0.889	6.604	7.493	2575.6	30.814	346.62
400.00	1.064	7.215	8.279	2886.1	31.275	425.48
425.00	1.545	8.662	10.207	3681.2	32.310	656.67
450.00	2.079	10.001	12.080	4500.4	33.205	935.36
475.00	2.653	11.243	13.896	5340.6	33.989	1260.2
500.00	3.259	12.398	15.658	6199.1	34.683	1629.7
550.00	4.541	14.480	19.021	7963.8	35.862	2497.5
600.00	5.881	16.303	22.184	9781.9	36.833	3528.4
650.00	7.251	17.915	25.165	11645.	37.654	4712.9
700.00	8.632	19.351	27.982	13545.	38.363	6042.3
750.00	10.012	20.639	30.651	15479.	38.985	7508.7
800.00	11.381	21.804	33.185	17443.	39.540	9105.1
850.00	12.735	22.862	35.597	19433.	40.041	10825.
900.00	14.070	23.829	37.899	21446.	40.498	12663.
950.00	15.383	24.718	40.100	23482.	40.919	14613.
1000.00	16.671	25.538	42.209	25538.	41.309	16671.
1050.00	17.936	26.297	44.233	27612.	41.675	18833.
1100.00	19.176	27.004	46.180	29705.	42.018	21094.
1150.00	20.391	27.664	48.055	31814.	42.343	23450.
1200.00	21.582	28.282	49.864	33939.	42.652	25898.
1250.00	22.748	28.863	51.611	36079.	42.947	28435.
1300.00	23.891	29.410	53.301	38233.	43.230	31058.
1350.00	25.011	29.927	54.938	40402.	43.502	33764.
1400.00	26.108	30.417	56.525	42583.	43.764	36551.
1450.00	27.183	30.881	58.065	44778.	44.017	39416.
1500.00	28.238	31.323	59.561	46985.	44.263	42357.
1550.00	29.272	31.745	61.016	49204.	44.502	45371.
1600.00	30.286	32.147	62.433	51435.	44.735	48458.
1650.00	31.281	32.532	63.813	53678.	44.962	51614.
1700.00	32.258	32.901	65.159	55931.	45.184	54838.
1750.00	33.217	33.255	66.472	58196.	45.402	58129.
1800.00	34.158	33.595	67.754	60471.	45.615	61485.
1850.00	35.083	33.923	69.006	62757.	45.824	64904.
1900.00	35.992	34.239	70.231	65054.	46.030	68385.
1950.00	36.886	34.544	71.429	67360.	46.232	71927.
2000.00	37.764	34.838	72.602	69677.	46.431	75528.
2050.00	38.628	35.124	73.751	72003.	46.628	79187.
2100.00	39.477	35.400	74.877	74339.	46.822	82903.
2143.00	40.197	35.631	75.828	76356.	46.986	86143.

H^o_{298} AND S^o_{298} APPLY TO THE REFERENCE STATE OF THE SOLID AT 298.15 DEG K

U. S. DEPARTMENT OF COMMERCE
Luther H. Hodges, *Secretary*

NATIONAL BUREAU OF STANDARDS
A. V. Astin, *Director*

THE NATIONAL BUREAU OF STANDARDS

The scope of activities of the National Bureau of Standards at its major laboratories in Washington, D.C., and Boulder, Colorado, is suggested in the following listing of the divisions and sections engaged in technical work. In general, each section carries out specialized research, development, and engineering in the field indicated by its title. A brief description of the activities, and of the resultant publications, appears on the inside of the front cover.

WASHINGTON, D. C.

Electricity. Resistance and Reactance. Electrochemistry. Electrical Instruments. Magnetic Measurements. Dielectrics. High Voltage.

Metrology. Photometry and Colorimetry. Refractometry. Photographic Research. Length. Engineering Metrology. Mass and Scale. Volumetry and Densimetry.

Heat. Temperature Physics. Heat Measurements. Cryogenic Physics. Equation of State. Statistical Physics.

Radiation Physics. X-ray. Radioactivity. Radiation Theory. High Energy Radiation. Radiological Equipment. Nucleonic Instrumentation. Neutron Physics.

Analytical and Inorganic Chemistry. Pure Substances. Spectrochemistry. Solution Chemistry. Standard Reference Materials. Applied Analytical Research. Crystal Chemistry.

Mechanics. Sound. Pressure and Vacuum. Fluid Mechanics. Engineering Mechanics. Rheology. Combustion Controls.

Polymers. Macromolecules: Synthesis and Structure. Polymer Chemistry. Polymer Physics. Polymer Characterization. Polymer Evaluation and Testing. Applied Polymer Standards and Research. Dental Research.

Metallurgy. Engineering Metallurgy. Microscopy and Diffraction. Metal Reactions. Metal Physics. Electrolysis and Metal Deposition.

Inorganic Solids. Engineering Ceramics. Glass. Solid State Chemistry. Crystal Growth. Physical Properties. Crystallography.

Building Research. Structural Engineering. Fire Research. Mechanical Systems. Organic Building Materials. Codes and Safety Standards. Heat Transfer. Inorganic Building Materials. Metallic Building Materials.

Applied Mathematics. Numerical Analysis. Computation. Statistical Engineering. Mathematical Physics. Operations Research.

Data Processing Systems. Components and Techniques. Computer Technology. Measurements Automation. Engineering Applications. Systems Analysis.

Atomic Physics. Spectroscopy. Infrared Spectroscopy. Solid State Physics. Electron Physics. Atomic Physics.

Instrumentation. Engineering Electronics. Electron Devices. Electronic Instrumentation. Mechanical Instruments. Basic Instrumentation.

Physical Chemistry. Thermochemistry. Surface Chemistry. Organic Chemistry. Molecular Spectroscopy. Molecular Kinetics. Mass Spectrometry.

Office of Weights and Measures.

BOULDER, COLO.

Cryogenic Engineering Laboratory. Cryogenic Equipment. Cryogenic Processes. Properties of Materials. Cryogenic Technical Services.

CENTRAL RADIO PROPAGATION LABORATORY

Ionosphere Research and Propagation. Low Frequency and Very Low Frequency Research. Ionosphere Research. Prediction Services. Sun-Earth Relationships. Field Engineering. Radio Warning Services. Vertical Soundings Research.

Radio Propagation Engineering. Data Reduction Instrumentation. Radio Noise. Tropospheric Measurements. Tropospheric Analysis. Propagation-Terrain Effects. Radio-Meteorology. Lower Atmosphere Physics.

Radio Systems. Applied Electromagnetic Theory. High Frequency and Very High Frequency Research. Modulation Research. Antenna Research. Navigation Systems.

Upper Atmosphere and Space Physics. Upper Atmosphere and Plasma Physics. Ionosphere and Exosphere Scatter. Airglow and Aurora. Ionospheric Radio Astronomy.

RADIO STANDARDS LABORATORY

Radio Physics. Radio Broadcast Service. Radio and Microwave Materials. Atomic Frequency and Time-Interval Standards. Millimeter-Wave Research.

Circuit Standards. High Frequency Electrical Standards. Microwave Circuit Standards. Electronic Calibration Center.

NBS