Preliminary Report
on the Thermodynamic Properties of
Selected Light-Element and
Some Related Compounds

(Supplement to NBS Reports 6297, 6484, 6645, 6928, 7093, 7192, 7437, 7587, and 7796)

1 July 1963

U.S. DEPARTMENT OF COMMERCE
NATIONAL BUREAU OF STANDARDS

THE NATIONAL BUREAU OF STANDARDS

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

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U.S. DEPARTMENT OF COMMERCE
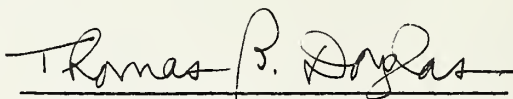### LUTHER H. HODGES, Secretary
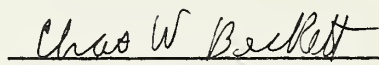## NATIONAL BUREAU OF STANDARDS

ABSTRACT

This is the tenth 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 compounds of primary interest in high-temperature research. The experimental part of the program is devoted mainly to an investigation of the simpler compounds in which Be, Al, and/or Li are combined with H, O, N, F, and/or Cl.

First are outlined, for each of the ten groups currently active in the program, the accomplishments during the past year and the research plans for the next year.

The results of three recent literature reviews are given. One review comprises the critical analysis of the low-temperature heat-capacity data for 22 light-element substances; their values of $S°_{298}$ and thermodynamic functions from $0°$ to $300°K$ were derived and are tabulated. The results of another review consists of a bibliography, presented without critical analysis, of recent publications of thermal data on aluminum compounds, beryllium compounds, and lithium fluoride. A third review presents a critical analysis of the available information on the heat of formation of beryllium fluoride, and an extensive survey of the information on its crystalline forms.

Several recent NBS experimental investigations are reported. In one, mass-spectrometric data on the vaporization of a preliminary sample of beryllium fluoride between $705°$ and $819°K$ are presented. The $BeO-BeF_2$ system also is under mass-spectrometric study at high temperatures; preliminary results have tentatively identified the molecule Be_2OF_2 and given an approximate value for its heat of formation. The rate of dissociation of $N_2F_4(g)$, as determined by a shock-wave method, is reported and discussed. Using the recently developed high-temperature microwave spectrometer, the microwave spectrum of lithium chloride was observed; these data and the molecular constants derived from them are presented.

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ii

TABLE OF CONTENTS

TABLE OF CONTENTS (continued)

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 data assembly will be consolidated, more critically evaluated in most cases, 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, C, and B. 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). Because the importance of a given substance to propulsion efficiency depends on a simultaneous combination of various thermodynamic properties, the NBS plans for experimental work are organized in such a way as to measure simultaneously as many as practical of the missing or poorly known thermodynamic properties of each substance of high priority.

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 described at some length in earlier semiannual reports of this series (see, e.g., NBS Report 7192 (1 July 1961) and NBS Report 7587 (1 July 1962)).

New NBS experimental results and literature compilations are presented in Part B of this report. In addition, a considerable amount of technical material of this nature is in a stage of approximation completion, but with sufficient need for further final treatment as to delay its presentation until the next semiannual report (1 January 1964).

1. THERMOCHEMISTRY

Summary of Research in

Experimental Thermochemistry of Light-Element Compounds

A. Measurements in Progress

1. Beryllium Oxide
Because of the importance of the value for the heat of formation of beryllium oxide in the thermochemistry of beryllium compounds, we have undertaken to redetermine it by direct combustion. Preliminary tests with metal of not-too-high purity indicated that slagging with the sample container was a serious problem. Beryllia crucibles have been obtained and as soon as samples of high-purity beryllium metal can be obtained, we shall continue our investigation. The oxide product will be retained for future characterization and study.

2. Perchlorates
Since our previous measurements on the heat of formation of $KClO_4$, there has appeared a series of measurements using electrical heating in which a different value for the ΔHf° of $KClO_4(c)$ was obtained. As this substance forms the reference from which our values for $NaClO_4$, $LiClO_4$ and NH_4ClO_4 were calculated, we are redetermining the heat of decomposition using a slightly varied procedure. These measurements are currently in progress.

We are also conducting measurements on the heat of formation of hydrazine diperchlorate, a sample of which has been obtained from the Reaction Motors Division of the Thiokol Chemical Corp. We are using the same general procedure as used for NH_4ClO_4; hence the result will be dependent on the value of ΔHf for $KClO_4$.

3. Beryllium chloride
We have temporarily suspended work on the heat of solution of beryllium chloride. The existence of more than one crystalline form has introduced additional uncertainties in the attempt to relate the heat-of-solution data to those obtained by direct chlorination of beryllium.

B. Future Measurements

1. Aluminum borohydride
We will undertake measurements of the heat of formation of $Al(BH_4)_3$ although our rotating bomb calorimeter is not yet completed. In view of

the difficulties reported with ordinary solution techniques, we will
attempt to obtain a satisfactory bomb reaction, possibly by use of a
hydrocarbon solution of the borohydride. Other procedures will also be
investigated, including a possible reaction with nitrogen, etc.

We will also continue with the study of the oxidation of beryllium
and complete our investigation of the perchlorates.

2. FLUORINE COMBUSTION CALORIMETRY

Progress during Fiscal Year 1963

A study of the energy of combustion and heat of formation of
aluminum carbide (Al_4C_3) was initiated in the second half of the year,
and good progress was made. The combustion is characterized by several
problems which determine the course of the research. The available sample
material is of about 95% purity. It has been used at NBS for heat-capa-
city measurements previously described in these reports, and has there-
fore been carefully characterized with respect to composition. Combus-
tion leads to a mass of corundum (alpha-Al_2O_3), as the principal solid
product, but a significant fraction of the product is in the form of
delta-Al_2O_3, which is more readily formed when carbon is present in the
combustion zone. The sample also contains some uncombined carbon, and
some aluminum nitride. The presence of refractory materials both in the
products and the starting materials renders the extent of reaction uncer-
tain. The most positive method to determine this is felt to be by analy-
sis of the product gases for CO_2. The presence of nitrogen in the sample
causes oxides of nitrogen to appear in the combustion products, probably
as NO_2. Because water in the bomb would tend to react with the Al_2O_3
formed, the reaction is carried out in anhydrous conditions. A method
has been developed for determining CO_2 and NO_2 in the combustion-product
gases. It involves the use of manganese dioxide to absorb NO_2 before the
gases pass into the CO_2 absorber.

Completeness of combustion is strongly influenced by the temperature
to which the reaction is allowed to go. The sample support, for instance,
becomes much hotter than when an organic material is burned, and the same
sample support system cannot be used for both benzoic-acid calibration
and the aluminum-carbide combustions. A sufficiently low-heat-capacity
platinum support to allow complete combustion of benzoic acid melts when
aluminum carbide is burned on it. On the other hand, incomplete combus-
tion of benzoic acid occurs if the support is massive enough to prevent
melting during aluminum-carbide combustions. The difference is attributed
to the fact that most of the heat, probably 95%, from a benzoic acid
combustion is carried away from the reaction by the products of combus-
tion, which are all gases. On the other hand, the solid product of alu-
minum-carbide combustion remains in contact with the sample support and
retains perhaps 50% of the heat at this location. The problem is solved
by the use of different supports for the two types of measurement.

The solid combustion products have been characterized by X-ray analysis.

The combustion calorimetry of beryllium has proceeded more slowly than was anticipated. Calorimeter-calibration experiments have been carried out, and the dust box for handling the beryllium and its combustion product, BeF_2, has been placed in service. Difficulties with leaks in the fluorine lines and valves, with the purity of the fluorine, and with some of the calorimeter control circuits have hindered progress. In addition it was necessary to be very careful in planning the method of characterizing the energy state of the combustion product, which is toxic and forms a glass not easily related to a standard crystalline state. A detailed literature study was made of the phase relations of BeF_2 and several fluoro-beryllates in order to elucidate this relationship.

In addition to the continuing surveillance on the liturature of the light-element compounds, a critical examination of the liturature on the heats of formation of the following fluorine compounds was made, and tentative new selections of best values were made: BeF_2, AlF_3, $AlF_3(H_2O)_3$, $AlF_3(H_2O)_{0.5}$, CF_4, ClF_3, F_2O, NH_4F, N_2F_2, N_2F_4, NF_2.

Plans for Fiscal Year 1964

At the present rate of progress of work on Al_4C_3 it is expected that measurements will be completed early in the fiscal year. The work on beryllium fluoride will be continued and completed, including the characterization of the energy state of the product obtained. A study will be initiated and carried out on the heat of formation of an alkali-metal fluoro-beryllate, probably Li_2BeF_4, on which no measurements have been made.

An experimental station for the combustion of gases in fluorine and the combustion of gaseous fluorine compounds has been planned, and preparations are in progress for putting it in active operation in the next few months. This calorimeter station is to be used for measuring the heat of formation of ClF_3 and possibly OF_2 or other volatile compounds of interest.

Critical literature reviews of heats of formation will be made on additional fluorine compounds, covering as rapidly as possible the light-element fluorides.

3. LOW-TEMPERATURE CALORIMETRY

This phase of the program is concerned with the accurate measurements of heat capacity between 15° and 400°K and with the calculations of thermal functions from the data. This experimental work is complemented by the analysis and calculation of thermal functions using the literature data on low-temperature heat capacity of substances of interest to the program. The results of the analysis are made compatible with the high-temperature enthalpy data, except where the data are extremely divergent.

High-speed digital computer programs are developed to perform the above analyses. Where data are unavailable or inadequate, efforts are made to obtain pure samples for experimental investigations.

Activity Summary - July 1, 1962 to June 30, 1963

Heat-capacity measurements on $BeO \cdot Al_2O_3$ (chrysoberyl) are almost completed. The results obtained thus far show that the heat capacity of $BeO \cdot Al_2O_3$ has the usual simple sigmoidal shape expected of a refractory solid of fairly high Debye characteristic temperature.

The measurements on Be_3N_2 (beryllium nitride) are also almost completed. Above about $330°K$ the sample of Be_3N_2 seemed to undergo some change. When heated above $330°K$, the subsequent measurements below this temperature gave results lower than those obtained prior to heating above this temperature. The change is considered to be caused possibly by moisture which could not be removed by pumping at high vacuum. A new chemical analysis will be needed on the sample when the measurements are completed.

Further calculations and correlation of the measurements completed on Al_4C_3 were performed. A paper on the thermodynamic properties of Al_4C_3 is in preparation.

The literature survey of low-temperature heat-capacity data was extended to include compounds of boron, nitrogen, sodium, potassium, mercury, titanium, and silicon in combination with hydrogen, oxygen, and the halogens. The data have been analyzed and the thermal functions from $0°$ to $300°K$ were calculated for $LiHF_2$, MgB_2, MgB_4, Na_2O_2, NaO_2, $NaNH_2$, $NaHF_2$, $NaBO_2$, $Na_2B_4O_7$ (crystal), $Na_2B_4O_7$ (glass), $KClO_3$, $KClO_4$, $KBrO_3$, KIO_3, $(NH_4)_2O$, NH_4OH, NH_4F, $NH_4F \cdot H_2O$, HNO_3, $HNO_3 \cdot H_2O$, $HNO_3 \cdot 3H_2O$, and HgO (red). Details of this analysis are given in another section of this report (Part B). Tables of thermal functions on other compounds of this group are still in preparation. They will be given in the subsequent reports.

Plans for the Period July 1, 1963 to September 30, 1964

Measurements in progress on $BeO \cdot Al_2O_3$ and Be_3N_2 will be completed.

About four to six of the following substances are expected to be investigated:
a.) $\underline{BeF_2}$
A high-purity sample in the glass state was received. A small portion of the sample was annealed at $400°C$ to gain experience in handling the material and to determine what equipment would be needed for annealing a larger amount of sample suitable for heat measurements. The plan is, at present, to anneal the sample directly in the calorimeter vessel. A platinum calorimeter vessel is expected to be delivered within a few weeks in which the BeF_2 sample will be annealed and the heat measurements made.

b.) BeO

The BeO sample, prepared for us by arc melting, appeared gray because of graphite inclusions. The gray coloration was removed by heating in a gas-fired furnace at 1750°C for about two hours. Measurements will be made to compare results obtained earlier on a sample of smaller crystallite size to determine whether surface effects are detectable.

c.) $LiBO_2$

This sample was prepared by fusing Li_2O and B_2O_3. Chemical analysis is being scheduled.

d.) Li_2BeF_4

A relatively small sample (about 25 cm^3) is on hand for measurements.

e.) Li_3AlF_6

A sample prepared by fusing LiF and AlF3 is available in the form of large "chunks". The material will require crushing to smaller sizes before chemical analysis and measurements can be made.

f.) $BeO \cdot 3Al_2O_3$

A sample prepared by arc fusion of stoichiometric amounts of BeO and Al_2O_3 was found by chemical analysis to be pure $BeO \cdot 3Al_2O_3$ within the limits of the chemical analysis.

g.) Other compounds of general interest to the program that are on hand are:

$Li_2O \cdot BeO$, $3BeO \cdot B_2O_3$, $Li_2O \cdot 2B_2O_3$, BeC_2, and Be_2B. No heat-capacity measurements have been found on these substances.

Literature analysis of other substances that should be of interest to the project will be continued.

4. HIGH-TEMPERATURE CALORIMETRY

This work includes all enthalpy measurements (heat capacities and heats of fusion and transition) above approximately room temperature, and uses the "drop" method exclusively, in connection with an ice calorimeter with the result that all measurements of enthalpy are relative to that at the ice-point (273°K).

During the past year measurements were completed on a sample of Li_2BeF_4 up to 873°K (about 140° above the melting point). On the basis of preliminary chemical analyses of the sample, the latter was found to contain a small excess of BeF_2 over nominal composition, and the considerable amount of resulting premelting was corrected for. The final analyses, not yet completed, differ substantially, so that the presentation of the final

corrected results and the corresponding thermodynamic functions will be deferred to the report to be issued six months from now.

Measurements from 273° to 1173°K on a preliminary sample of $BeO \cdot Al_2O_3$ had been completed earlier and a preliminary table of thermodynamic functions based on the results was issued a year ago (NBS Report 7587, Table B-83, p. 172). Since then a purer sample has become available, and measurements on it are nearly complete. The completed results will be smoothed with low-temperature heat-capacity measurements currently being completed (see preceding section), so that a revised table of thermodynamic functions will soon be available.

Enthalpy measurements (273° to 1173°K) are presently in progress on a sample of Li_3AlF_6 whose composition is stoichiometric within the precision of the chemical analyses. (An earlier attempt to measure this substance had to be abandoned because of leakage which all liquid fluoroaluminates seem to show.)

During the next fifteen months enthalpy measurements are planned on BeF_2 (crystalline if a sample in that form becomes available), $BeO \cdot 3Al_2O_3$, Be_2C, and possibly also on a sample of $BeO \cdot B_2O_3$ if a definite chemical compound proves to exist. These measurements will probably be confined to the temperature range 273° to 1173°K, particularly in the case of those substances which cannot be readily handled at higher temperatures. However, at present progress is being made toward making a second "drop method" apparatus operational, and this facility may yield some precise enthalpy data on Al_2O_3 up to 1800°K within the next year.

5.   COMPOUNDS OF THE LIGHT ELEMENTS

This section of the project was formed to engage in the synthesis and purification of materials needed by other groups. As the project progressed, the work of this group became more involved in the study of certain compounds of the light elements, a great part of which was classified.

During the past year studies have been made on the decomposition of certain light-element compounds by the Knudsen cell-mass spectrometer method and by gas-chromatography studies of the decomposition products. It was thought that some idea of the structure of the parent compound could be had from the decomposition products. Since this work is classified, a separate report has been prepared and is presently being reviewed.

The apparatus for the preparation of a single-phase crystalline beryllium fluoride by both the hydrofluothermal method and by the phase decomposition method has been built and is being tested. The work was delayed by the receipt of damaged equipment and by operational problems arising from the corrosive atmosphere at high temperatures.

Samples of trimethylhydrazine have been prepared and purified.

The literature survey on intermetallic compounds and alloys of the light metals has continued.

An apparatus for the purification and characterization of aluminum borohydride has been designed and parts are being built or acquired.

During the next year the preparation of the single-phase crystalline beryllium fluoride will be continued. Since the apparatus is essentially complete and only details remain to be corrected, the production of crystalline forms should begin shortly.

The purification and characterization of aluminum borohydride will be carried out in cooperation with the heat-measurement groups.

Miscellaneous preparative and purification work will be carried out as required by other groups in the project.

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

Analytical studies of the light-element compounds will continue.

6. LIGHT-ELEMENT EQUATION OF STATE

The Exploding Wire Project is an experimental program which was undertaken in order to explore the feasibility of employing electrical discharge techniques as the means for producing a high-temperature (between 2,000 and 6,000°K), high-pressure (up to 100 atm) system. The ultimate objective of the project is to determine, by experimental measurements, the equation of state of selected elements (Al, Be, Zr) under these extreme conditions. Thus far, the program has included: 1) the design, construction and instrumentation of the required experimental apparatus, 2) the exploration and development of techniques of high-speed measurement and high-speed photographic observation, and 3) a theoretical study of the hydrodynamic behavior of the exploding-wire system. The work on this program will continue during the next Fiscal Year (1964).

Activity Summary - July 1, 1962 to June 30, 1963

The work on the measurement of voltage, current and electrical energy under the extremely transient conditions of a high-energy electrical discharge continued during this period. A paper entitled "Calorimetric Calibration of the Electrical Energy Measurement In An Exploding Wire Experiment", which describes the techniques employed for these measurements, was published in Exploding Wires, Volume 2 (1962), p. 97. During the past six months, considerable effort was concentrated on a study of the errors involved in these measurements. Thus far, this study has indicated a need for a number of corrections in the measurements. This part of the work is now progressing at a faster pace, due to the addition of personnel.

In the area of design and construction, experimental setups for the calibration of the electrical energy input to the wire at 20 kv, 200 ka and 100 kc (intermediate range) and at 100 kv, 400 ka and 750 kc have been completed. Preliminary runs have been made at voltages up to 30 kv and frequencies up to 350 kc. The records from these experiments indicated serious difficulties with interference from the triggering circuits and with induced voltages in the voltage measuring circuit. Several new approaches to these problems are now being investigated.

The theoretical study of the hydrodynamic aspect of the exploding wire system did not progress as planned, due to the absence of key personnel.

Plans for Period July 1, 1963 to September 30, 1964

During this period, as time and personnel permit, efforts will be concentrated on the following tasks. 1) The study of the measurement errors involved in electrical measurements will continue, and will be extended to include measurements at the higher voltages and frequencies mentioned above. It is hoped that a more satisfactory technique for measuring the transient voltages during the discharge will be developed. 2) Several techniques for automatic reduction of the experimental data will be investigated. 3) The study of the hydrodynamic flow field will be completed. 4) With the addition of new personnel, time-resolved spectrographic studies of the exploding wire system will be initiated. 5) Preliminary experiments, in which tubular, conical and rectangular samples are heated, by electrical discharge, up to and beyond their melting points, will be conducted.

7.   SHOCK-WAVE KINETICS DATA

The rate of dissociation of tetrafluorohydrazine behind a shock wave has been determined for the temperature range 25 to 150°C at total pressures from 0.6 to 6 atm. The reaction, $N_2F_4 \rightleftarrows 2NF_2$, $\Delta H = 19.8 \pm 0.8$ kcal./mole, was carried out for 1 percent mixture of N_2F_4 in nitrogen and in argon, and its progress was followed by time-resolved spectrophotometric observation of the optical absorption of the difluoramino radical.

The results showed that, at 400°K, the reaction was quasi-unimolecular over the experimental pressure range, the experimentally determined activation energy being 19.0 kcal./mole. An extrapolation of the experimental first-order specific rate to infinite pressure was carried out and the result showed that the limiting first-order specific rate k^∞ may be expressed by the following Arrhenius type equation:

$$k^\infty = 2.3 \times 10^{15} \exp (19.8 \text{ kcal./mole/RT}) \text{ sec.}^{-1}$$

The high value of the pre-exponential term in this equation was explained on the basis of Eyring's transition state theory in terms of a loosely-bound structure for the activated complex in which free rotation occurs about the N-N bond.

A technical account of this work may be found in Part B of this Semi-Annual Report.

This research was sponsored by ARPA during the period 1 July 1961 to 1 March 1962.

8. HIGH-TEMPERATURE MICROWAVE SPECTROSCOPY

The original design for a high-temperature microwave spectrometer was abandoned after numerous technical difficulties developed. A novel and much simpler spectrometer has now been constructed and used successfully on several problems. This instrument has been operated at temperatures up to 1000°C, and the design is capable of extension to even higher temperatures. The present model allows the frequency range 30 - 60 kmc to be covered, although somewhat lower frequencies can be reached by slight modifications.

With this spectrometer it has been possible for the first time to detect the spectra of both AlCl and AlF. Accurate rotational constants have been derived for these molecules. From the conditions for appearance of the spectrum, some information has also been obtained on the heat of formation of AlF, although these measurements can be refined considerably. The spectrum of LiCl has also been measured and analysed.

During the next year the remaining details in the work on AlCl and AlF will be completed. Efforts will be made to observe spectrum of AlF_2 and $AlCl_2$ (although there is no indication of the presence of these species in the systems studied so far). Following this the major effort will be devoted to the hydroxides, oxides, and metaborates of lithium and the other alkali metals. It is hoped that spectra can be detected in some of these compounds which will allow structural trends to be established.

9. HALIDE SOLID-VAPOR EQUILIBRIA (TRANSPIRATION METHOD)

During the past year the uniformity of temperature and its accuracy of measurement in the vaporization cell of the new high-temperature transpiration apparatus were improved. Seventeen successful measurements (in dry argon) of the vapor pressure of AlF_3 were then made in the ranges 1233° to 1288°K and 3 to 9 mm Hg. (The stoichiometric composition of the sample was verified within the precision of the chemical analysis: %Al, ± 0.02%; %F, ± 0.12%.) A Third-Law treatment of the values indicated no detectable trend with temperature of the standard heat of sublimation, from which a value for the standard heat of formation of $AlF_3(g)$ can be calculated. The results were of sufficiently high precision as to indicate, when compared with six other sets of published vapor-pressure values for AlF_3 (various methods and temperature ranges), that the saturated vapor probably contains several percent of the dimer (Al_2F_6). This result is consistent with direct observations of the vapor in mass-spectrographic studies reported by another Laboratory. The foregoing NBS results and conclusions were described in detail in the preceding semiannual report (NBS Report 7796, 1 January 1963, pp. 157-171).

The above work on pure AlF_3 was followed by preparations for similiar work to study two gaseous systems, AlF_3-$AlCl_3$ and AlF_3-HF. The experimental procedure will consist of passing argon containing a known proportion of the more volatile component ($AlCl_3$ or HF) over solid AlF_3 in order to determine how much extra AlF_3 evaporates because of partially completed chemical reaction with the reactive gas. Heats of reaction can be calculated from such data at different temperatures.

A series of calculations was carried out to ascertain the probable conditions under which the various species which may form are most likely to be identified and their properties evaluated from the raw data. Modifications of the existing transpiration apparatus were then designed and placed in the shops for construction. At present these modifications are specifically for the AlF_3-$AlCl_3$ system, and consist principally of inserting into the flow system suitable units to protect the $AlCl_3$ from contamination, to evaporate it at constant known temperatures, and to determine the amounts which have passed over the AlF_3. Subject to receipt of some ordered parts, expected soon, the modified apparatus should be ready for preliminary tests and some initial runs shortly.

It is planned to carry out series of measurements on the above two systems during the next fifteen months.

10. VAPORIZATION OF REFRACTORY SUBSTANCES

Some details of the experimental approach to the study of the vaporization of light-metal oxides and other compounds were presented in the Eighth Technical Summary Report, NBS Report 7587, page 55 (July 1, 1962). In a chapter of Part B of the present report a more detailed account of results obtained during the past year on one part of this activity is given.

Activity during the past year may be briefly summarized as follows: Investigations of the BeF_2, BeF_2-BeO, and BeO-Al_2O_3 systems have continued, and those concerned with the first two of the systems have been brought nearly to the stage of completion. The study of the second system required the development of a temperature-gradient effusion cell, as discussed in the above Eighth Summary Report. In particular, this cell was used with the direction-focussing mass spectrometer for the study of the reaction: $BeO(c) + BeF_2(g) \rightarrow Be_2OF_2(g)$.

Studies of the free vaporization of Al_2O_3 in vacuum and in the presence of other gases have been largely suspended during the year pending the development of a more direct, but instrumentally more sophisticated experimental approach. Considerable effort has been devoted to the adaptation of a photoelectric pyrometer for recording temperatures in the arc image furnace used for these studies. The possibility of employing a small mass spectrometer with the furnace to identify vapor species has also been explored, and a quadrupole mass filter, adapted for solids analysis, has been ordered. Delivery of this item is overdue, but the instrument should be received shortly.

-11-

Program Plans, July 1, 1963 - September 30, 1964

During the next fifteen months, it is planned to continue the study of the chemical systems mentioned above, using the experimental approaches previously described. As time permits, the study of additional light-element compounds will be commenced as indicated in the following summary of plans.

1. Mass spectrometric measurements of the vapor pressure of the $BeO-BeF_2$ system will be completed and reported.

2. The vapor phase of the $BeO-Al_2O_3$ system will be studied with the mass spectrometer and related to the composition of the solid-liquid phases.

3. An exploratory investigation of the BeF_2-BeCl_2 system will be started.

4. The kinetics of vaporization of some of the above systems may be undertaken with a time-of-flight mass spectrometer.

5. The quadrupole mass filter will be adapted for use with the arc-image furnace for the study of the free evaporation of Al_2O_3 in vacuum and in the presence of water vapor.

PART B. THERMODYNAMIC PROPERTIES OF LIGHT-ELEMENT COMPOUNDS

Chapter B-1

THE MICROWAVE SPECTRUM OF LITHIUM CHLORIDE

by David R. Lide, Jr.

Introduction

Accurate rotational constants have been obtained for all of the alkali halide molecules except lithium chloride, either by conventional microwave spectroscopy or by molecular beam techniques. The microwave spectrum of lithium chloride has now been observed on the recently-constructed high-temperature microwave spectrometer at the National Bureau of Standards. The principal rotational constants of LiCl have been determined, and from a combination of microwave and molecular beam electric resonance data, the variation of dipole moment with vibrational state has been measured.

The spectrum of LiCl has also been observed by P. Cahill and L. P. Gold of Columbia University. Their results are in close agreement with those described here.

Experimental

The spectrometer used in this investigation consists of a waveguide made of stainless steel contained in a quartz vacuum jacket which is heated over a one-foot region in the center by an external furnace. The waveguide is of the "split" variety; its internal dimensions are 5 mm x 20 mm, with a slot in each of the narrow faces (Fig. 1). Stark modulation at 80 kc is applied between the two halves. The Stark selection rule is thus $\Delta M = \pm 1$; with the present 4:1 ratio of height to width, the Stark field is sufficiently uniform to give well-resolved components. Since there is no dielectric within the microwave field region, the transmission is excellent at high temperatures and at high microwave frequencies. Aside from the waveguide, the spectrometer is a conventional Stark-modulation instrument. The microwave source was a QK 293 klystron; frequency measurements were made by comparison with harmonics of a 1000 Mc frequency standard which was locked to WWV.

Spectrum and Molecular Constants

The $J = 0 \to 1$ transitions of the first three vibrational states of Li^7Cl^{35} and of the first two states of Li^7Cl^{37} have been observed in the 42 kmc region at a temperature of 600 - 800°C. The measured frequencies are listed in Table I. No nuclear quadrupole hyperfine structure was resolved. From molecular beam results[1] on Li^6Cl, one can show that the

hfs from Li^7 is extremely small, while that from Cl^{35} and Cl^{37} should give maximum splittings of the order of 0.7 Mc, which is slightly below the resolution obtained in these measurements. However, further calculations indicate that the peak of the unresolved hyperfine triplet should lie within $\pm$ 0.1 Mc of the center frequency. Consequently, no corrections for hfs have been applied.

The frequencies have been analyzed by the usual Dunham method.[2] The frequencies f_v for the $J = 0 \rightarrow 1$ transition in the $v = 0$, 1, and 2 states are given by

$$f_0 = 2Y_{01} + 4Y_{02} + Y_{11} + (1/2)Y_{21}$$

$$f_1 = 2Y_{01} + 4Y_{02} + 3Y_{11} + (9/2)Y_{21}$$

$$f_2 = 2Y_{01} + 4Y_{02} + 5Y_{11} + (25/2)Y_{21}.$$

Since no experimental value for the centrifugal distortion constant $Y_{02} \approx -D_e$ is available, it has been estimated from the relation $D_e = 4B_e^3/\omega_e^2$. Using the value of ω_e reported by Klemperer, et al.,[3] and a B_e derived from an approximate treatment of the microwave data, we obtain $D_e = 0.10$ Mc, which is sufficiently accurate for the present purposes. The remaining Dunham coefficients obtained by solving the above set of equations are listed in Table 1. For Li^7Cl^{37}. where only two frequencies are available, the Y_{21} coefficient was calculated from that of Li^7Cl^{35} by means of its theoretical mass-dependence.[2]

The constants for the two isotopic species are in excellent agreement. The ratio $B_e(Li^7Cl^{35}):B_e(Li^7Cl^{37})$ is found to be 1.009109 $\pm$ 0.000010, which compares with the ratio 1.009110 of the reciprocals of the reduced masses.[4] The corresponding ratio for α_e is 1.0139 $\pm$ 0.0016, in good agreement with the theoretical value of 1.0137. It is interesting that α_e and γ_e fall quite close to the empirical curves proposed by Green and Lew[5] for the alkali halides; the values obtained by extrapolating their curves are $\alpha_e = 245$ Mc and $\gamma_e = 1.17$ Mc. From the Morse-function relationship,

$$\alpha_e = 6(B_e^2/\omega_e) \left[(\omega_e x_e/B_e)^{\frac{1}{2}} - 1 \right]$$

we obtain $\alpha_e = 200 \pm 15$ Mc with the aid of the infrared values[3] of ω_e and $\omega_e x_e$. Green and Lew[5] have pointed out that the Morse function gives consistently low values of α_e for the alkali halides.

With this work, the determination of the principal rotational constants of the alkali halides by microwave measurements is complete. We therefore present in Table III a summary of these data.

Potential Constants

The Dunham treatment is based on the expansion of the potential energy as a power series in $\xi = (r - r_e)/r_e$:

$$U(\xi) = a_0\xi^2 (1 + a_1\xi + a_2\xi^2 + \ldots)$$

The relationships between the potential constants a_n and the coefficients $Y_{\ell j}$ are given in Reference 2. Combination of the present microwave results with the values $\omega_e = 641 \pm 3$ cm^{-1} and $\omega_e x_e = 4.2 \pm 0.3$ cm^{-1} which have been obtained from the infrared spectrum[3] permits the following constants to be determined:

$$a_0 = (4.36 \pm 0.04) \times 10^9 \text{ Mc}$$

$$a_1 = -2.72 \pm 0.01$$

$$a_2 = 5.3 \pm 0.4$$

The a_3 constant can in principle be calculated from $Y_{21} \approx \gamma_e$. However, the value obtained ($a_3 = -9 \pm 3$) is subject to a large cumulative uncertainty from the errors in a_1 and a_2, and the contribution of the experimental Y_{21} term is actually less than this uncertainty. It is interesting that the value of a_1 for LiCl is almost identical with those of the other lithium halides (-2.70, -2.71, -2.70 in LiF, LiBr, and LiI, respectively).[6,7]

The Dunham correction[2] to B_e, $B_e = Y_{01}\left[1 - (B_e^2/\omega_e^2)\beta_{01}\right]$, is usually of the order of 1 part in 10^5 in molecules of this type. With the presently available constants this correction is found to be 0 ± 0.2 Mc; the chief source of uncertainty is the rather poor value of $\omega_e x_e$.

Internuclear Distance

The value of r_e, the equilibrium internuclear distance, was obtained from B_e through the relation

$$B_e = h^2/2\mu r_e^2$$

where μ is the reduced mass of the molecule. If atomic masses[4] are used to evaluate μ the result is

$$r_e = 2.02067 \pm 0.00006 \text{ A}^\circ$$

where the error is due almost entirely to the error in Planck's constant and the atomic mass unit.[8] A calculation of the internuclear distance using ionic rather than atomic masses gives a change in r_e of $+0.00005$ A$^\circ$; Since lithium chloride is not 100% ionic ($\mu_0/er_e = 0.7$) the actual effect on r_e of the ionic nature of the molecule is less than the error in r_e. In the absence of a measurement of the rotational magnetic moment of lithium chloride, no correction of r_e for electronic motion[9] was attempted.

Several empirical estimates based on additivity of ionic radii have been made of internuclear distances in alkali halides. Honig et al[9] predicted values of r_e which were 2% high for KF[5] and 2% low for LiF;[8] their predicted value of $r_e = 2.022$ A$^\circ$ for LiCl is in excellent agreement with the present result, however. Krasnov,[10] using a similar model, was able to fit the then known alkali halide distances to a mean deviation of $\pm.003$A$^\circ$. His calculated r_e for KF agreed with experiment within .005A$^\circ$ but his error was .020 A$^\circ$ for LiF and .017A$^\circ$ for LiCl.

Dipole Moment

Stark-effect measurements were made at N.B.S. as additional confirmation of the assignment of the spectrum; they also confirmed the expected agreement of the dipole moments of Li^7Cl^{35} and Li^7Cl^{37} within the experimental precision of about 1%. These measurements did not permit a very good absolute determination of the dipole moment because of the difficulty in accurately measuring the Stark-field spacing at the operating temperature. However, very reliable dipole moment values may be obtained by combining the present rotational constants of Li^7Cl with the molecular beam measurements of Marple and Triska[1] on the Li^6Cl species. With the aid of the well-known dependence[2] of B_e, α_e and γ_e on reduced mass,[4] we calculate $B_e = 24116.6$, $\alpha_e = 291.8$, $\gamma_e = 1.6$ Mc for Li^6Cl^{35} and $B_e = 23925.4$, $\alpha_e = 288.3$, $\gamma_e = 1.6$ for Li^6Cl^{37}. Thus the B_v values for Li^6Cl^{35} and Li^6Cl^{37} may be calculated with an accuracy of 1 Mc or better, and the combination of these with the μ_v^2/B_v results of Marple and Trishka lead to accurate values of μ_v. The results of this calculation are presented in Table II.

The variation of dipole moment with vibrational state is linear within the experimental precision; it may be expressed by the formula (for Li^6Cl^{35}):

$$\mu_v = 7.075 + 0.0885 \ (v + \tfrac{1}{2}) \ D.$$

This variation with v implies a difference of less than 0.001 D between the moments in corresponding states of Li^6Cl^{35} and Li^6Cl^{37}. It is seen from Table II that the agreement is excellent.

The first dipole derivative may be estimated by making the usual expansion of μ abour r_e to obtain

$$\mu_v = \mu_e + (\partial\mu/\partial r)_e \ \langle r - r_e \rangle + \ldots$$

To a first approximation the average distance is given by

$$\langle r - r_e \rangle = -(3a_1 r_e B_e/\omega_e) \ (v + \tfrac{1}{2})$$

where a_1 is the Dunham coefficient given above. If we assume that all terms in the dipole-moment expansion beyond the linear one can be neglected, we obtain

$$(\partial\mu/\partial r) = 4.6 \ D/A°$$

As in the other alkali halides which have been studied, the sign of $(1/\mu) \ (\partial\mu/\partial r)$ is positive. It should be emphasized that the dipole-derivative obtained in this way is subject to some uncertainty because of the neglect of the $\partial^2\mu/\partial r^2$ term, which enters in the same order as $\partial\mu/\partial r$.

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Table I. Observed frequencies $(J = 0 \rightarrow 1)$ and derived constants[a] for Li^{7}Cl.

Vibrational State	Li^{7}Cl^{35}	Li^{7}Cl^{37}
$v = 0$	42122.2 ± 0.2 Mc	41743.1 ± 0.2 Mc
$v = 1$	41646.6 ± 0.2	41274.1 ± 0.2
$v = 2$	41175.8 ± 0.2	...
$Y_{01} \approx B_e$	21181.1 ± 0.1[b]Mc	20989.9 ± 0.1[b]
$-Y_{11} \approx \alpha_e$	240.2 ± 0.2	236.9 ± 0.2
$Y_{21} \approx \gamma_e$	1.2 ± 0.2	(1.2)[c]
r_e	2.02067 ± 0.00001Å[d]	2.02067 ± 0.00001Å[d]

[a]A calculated value of $D_e = 0.10$ Mc has been used in the data reduction.
[b]With the presently available molecular constants, the Dunham correction to Y_{01} is 0 ± 0.2 Mc; thus an additional uncertainty of ± 0.2 Mc should be assigned to B_e.
[c]Calculated value.
[d]This uncertainty in r_e includes only the contribution of experimental uncertainties in the present data. See text for discussion of other sources of error.

Table II. Electric dipole moment of Li^{6}Cl.

State	Li^{6}Cl^{35}	Li^{6}Cl^{37}
$v = 0$	$7.119_5 \pm 0.0006$[a] D	$7.119_2 \pm 0.0008$
$v = 1$	$7.206_9 \pm 0.0008$	$7.207_1 \pm 0.0012$
$v = 2$	$7.296_4 \pm 0.0012$	$7.297_2 \pm 0.0014$
$v = 3$	$7.386_5 \pm 0.0018$	...

[a]The uncertainties are derived from estimates of random errors given in Reference 1. This reference cites an additional systematic error of ± 0.0022 D.

Table III. Rotational constants and internuclear distances of the alkali halides

Molecule	B_e (Mc)	$\alpha_e{}^*$ (Mc)	$\gamma_e{}^*$ (kc)	r_e (Å)	Ref.
Li^6F	45231.0149 ± .007	722.3089 ± .005	5827.0 ± 5.0	1.563892 ± .00005	g
Li^7Cl^{35}	21181.1 ± 0.1	240.2 ± 0.2	1200 ± 200	2.02067 ± .00006	h
Li^7Br^{79}	16650.179 ± 1.10	169.09 ± 0.08	656 ± 40	2.17042 ± .00004	a,i
Li^7I^{127}	13286.15 ± 0.10	122.62 ± 0.10	455 ± 50	2.39191 ± .00004	a,i
NaF	13098.230 ± .034	136.660 ± .024	698 ± 10	1.92593 ± .00006	f
$NaCl^{35}$	6537.07 ± 0.10	48.28	145	2.3606 ± .0001	i,c
$NaBr^{79}$	4534.4658 ± .0072	28.2091 ± .0038	72.92 ± 1.2	2.50201 ± .00004	a
NaI^{127}	3531.7187 ± .0072	19.4198 ± .0052	42.9 ± 1.6	2.71143 ± .00004	a
$K^{39}F$	8392.482 ± .070	69.991 ± 0.01	204 ± 5	2.17144 ± .00005	b
$K^{39}Cl^{35}$	3856.399 ± .007	23.680 ± .001	50 ± 1	2.6666 ± .0001	d,c
$K^{39}Br^{79}$	2434.945 ± .002	12.136 ± .001	23 ± 1	2.82075 ± .00005	a,k
$K^{39}I^{127}$	1824.9778 ± .0014	8.0272 ± .0015	11.62 ± 0.39	3.04781 ± .00005	a
$Rb^{85}F$	6315.639 ± .036	45.638 ± .017	94 ± 7	2.26554 ± .00005	e
$Rb^{85}Cl^{35}$	2627.414 ± .010	13.601 ± .005	21 ± 2	2.78670 ± .00006	j
$Rb^{85}Br^{79}$	1424.8522 ± .0016	5.5760 ± .0012	6.83 ± 0.32	2.94471 ± .00005	a
$Rb^{85}I^{127}$	984.3062 ± .0024	3.28156 ± .0017	3.53 ± 0.25	3.17684 ± .00005	a
CsF	5527.34 ± .04	33.13 ± .05	9 ± 12	2.3453 ± .0001	i
$CsCl^{35}$	2161.208 ± .015	10.085 ± .004	7.1 ± 0.7	2.9062	i,c
$CsBr^{79}$	1081.3333 ± .0022	3.72052 ± .00040	3.234 ± .044	3.07221 ± .00005	a
CsI^{127}	708.32904 ± .00090	2.04638 ± .00057	1.482 ± .082	3.31515 ± .00006	a

References for Table III

*   The corresponding Dunham constant has been given in some cases.

a. Reference 7

b. Reference 5

c. See also P. Clouser and W. Gordy, Bull. Am. Phys. Soc. $\underline{8}$, 326 (1963).

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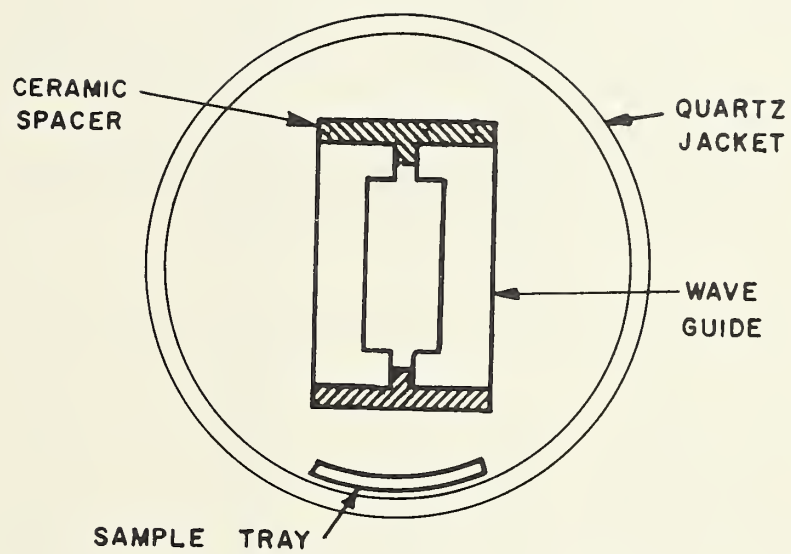
Fig. 1. Cross-section of the N.B.S. high-temperature waveguide.

Chapter B-2

A BIBLIOGRAPHY RELATING TO HEATS OF FORMATION, ENTHALPY CHANGES RESULTING
FROM PHASE CHANGES, AND THE HEAT CAPACITIES OF ALUMINUM AND BERYLLIUM
FLUORIDES, OXYFLUORIDES, CHLORIDES, AND OXYCHLORIDES, AND OF LITHIUM FLUORIDE

by John E. Neufer

The numbers in the body of Table 1 designate the references treat-
ing the compound and property indicated by the row and column headings.
This bibliography attempts to consolidate all the pertinent references
from NBS Report 6297 dated Jan. 1, 1959 (Chap. 2, 3, and 5), NBS Report
7192 dated July 1, 1961 (Chap. 5, 7, and 8), and NBS Report 7796 dated
Jan. 1, 1963 (Chap. 2, 3, and 6). It has been supplemented by a search
of the following.
   1. Chemical Abstracts: 1957 thru mid-year 1962 (via indices)
   2. Chemical Titles from January 1961 thru June 1963.
   3. The Armed Services Technical Information Agency Abstracts from
      January 1961 thru June 1963 (via indices).

TABLE I

Aluminum Compounds

	ΔH°_f[1]	ΔH_p[2]	ΔH of reaction	H°_T	Vapor Pressure	Other
AlCl(c)	29		89	75		
(g)	97		63, 112	68, 106, 144		
AlCl₂(c)	29					
AlCl₃(c)	5		63, 89, 107	7, 106		75
(l)		2				
(g)		61		144		67, 71, 108
)x 3	48, 49, 58		108			
AlOCl(c)	58			129		
AlF(c)hyp[4]	6, 8, 70				35	4
(g)hyp[4]	8, 10, 11, 16, 19, 20, 23, 25, 28, 47, 51, 77, 78, 90, 94, 96, 97, 95, 101, 102, 111, 114, 127		36, 112, 120	68, 106, 144	111	
AlF₂(c)hyp[4]	11, 69					
(g)hyp[4]	70, 78, 101, 102, 114					
AlF₃(c)	1, 8, 16, 18, 22, 23, 24, 33, 37, 39, 69, 76, 77, 78, 90, 96, 101, 102, 114, 123, 124, 127, 137	41, 141	23, 39, 76, 77, 120, 123, 124, 140	3, 40, 79, 106, 119, 121	35, 74, 92, 93, 94	
(l)		41				
(g)	69, 78, 90, 95, 96, 101, 102	4, 16, 71, 73, 92, 93, 94, 121	108	144	92	
)x 3						
AlOF(g)	145					67

TABLE I (continued)

Beryllium Compounds

	$\Delta H_f^{\circ}1$	$\Delta H_p^{\,2}$	ΔH of reaction	H_T°	Vapor Pressure	Other
BeCl(c)	91			106, 144		44
(g)						
BeCl$_2$(c)	13, 122, 142		122, 143	118		52, 83, 100
(l)						44, 46, 133
(g)	126, 135	109		132, 144		44, 46
)x^3		109				
BeF(c)	25			113	54	
(g)	10, 19, 38, 62, 69, 70, 78, 90, 101, 102, 114, 127, 146			106, 144		44
BeF$_2$(c)	8, 37, 51, 69, 81, 90, 95, 96, 102, 130		81, 130		26, 80, 138	14, 52, 83
(l)					26, 42, 60, 80	
(g)	51, 69, 70, 78, 90, 95, 96, 101, 102, 114, 126, 127			144		44, 46, 98
)x^3						44

-24-

TABLE I (continued)

Lithium Fluoride

	ΔH_f°[1]	ΔH_p[2]	ΔH of reaction	H_T°	Vapor Pressure	Other
LiF(c)	5, 8, 16, 30, 31, 37, 51, 70, 78, 90, 96, 99, 101, 102, 114, 125, 127, 131	72	9, 17, 30, 74, 123, 125	11, 21, 57, 106, 113, 142	43, 50, 56, 59, 65, 66, 86, 103	15, 84
(1)	105	16, 21, 32, 34, 55, 117			87	
(g)	10, 19, 50, 70, 78, 85, 90, 96, 101, 102, 104, 127	16, 50, 56, 64, 65, 66, 72, 86, 104, 117	116	68, 115, 139, 143		98, 134, 136
)x[3]	50, 70, 78, 82, 96, 101, 102, 104, 114	50, 56, 65, 66, 71, 86, 117	53, 65, 86, 88	70, 113	45, 50, 56, 65, 66, 103, 110	27, 45, 69, 87, 88, 128, 134

1. Includes lattice and dissociation energies.
2. ΔH_p represents all enthalpy changes which accompany phase changes, i.e., heats of transition, fusion, vaporization, and sublimation.
3.)x refers to references concerned with dimers, trimers, etc.
4. "hyp" refers to a hypothetical compound.

-25-

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Chapter B-3

A DETERMINATION OF
THE RATE OF DISSOCIATION OF TETRAFLUOROHYDRAZINE BY A
SHOCK WAVE METHOD

by L. M. Brown

1. Introduction

An experimental investigation of the rate of dissociation of tetra-fluorohydrazine has been made by a shock wave method[1]. This compound, N_2F_4, was discovered recently by Colburn and his co-workers[2] and shown[3] to dissociate reversibly to the stable difluoramino radical according to the equilibrium equation, $N_2F_4 \rightleftarrows 2NF_2$. The enthalpy of dissociation is 19.8 ± 0.8 kcal./mole[4] independent of temperature in the range, $25°$ to $150°C$.

Aside from the importance of N_2F_4 and NF_2 in chemical synthesis[5], these compounds are also of interest by virtue of the elementary character of the molecule-radical equilibrium which exists between them. For many years kineticists have focussed attention on the rates of elementary processes because of the important role they play in the majority of chemical reactions. Although many of the properties of N_2F_4 and NF_2 have been investigated[5,6], no data had been reported[7], at the start of this research, on the rate of the dissociation reaction. Hence, it seemed desirable to obtain such data experimentally and at the same time to investigate the mechanism of the dissociation.

2. Outline of the Experimental Method

The experimental method consisted of the observation of the approach to dissociation equilibrium in 1 percent mixtures of N_2F_4 in nitrogen and in argon behind weak incident shock waves (Mach 1.2 to 1.6) generated in a shock tube. The progress of the reaction was monitored by a time-resolved spectrophotometric technique in which the decrease of the transmission of radiation of 2602A wavelength (due to absorption by NF_2[3]) was observed. A value of 537 ± 46 liters/mole cm. for the absorption coefficient of NF_2 was determined experimentally. Details of the apparatus and experimental method were given in a previous NBS Report to ARPA[5].

3. Results and Discussion

Experiments were carried out for temperatures in the range, $343°$ to $410°K$ at pressures between 0.6 and 6 atm. The experimental first order specific rate was found to be less than first order in the diluent gas concentration at $400°K$, a dependence which, in the case of nitrogen, diminished with increasing total pressure. This behavior is typical of a unimolecular process carried out at pressures intermediate to its low- and high-pressure limits where, respectively, second order and first order kinetics prevail. The temperature dependence of the specific rate of this

quasi-unimolecular process in nitrogen, for total pressures near 2 atm., is given by the Arrhenius type equation, $k = 5.4 \times 10^{14}$ exp (-19.0 kcal./mole/RT) sec.$^{-1}$. A method developed by Johnston[9] was employed as a means for obtaining estimates of the limiting low- and high-pressure specific rates from the experimental data. The lower limit of the low-pressure second order specific rate was found by this method to be 2×10^6 liters/mole sec. at 400°K. The estimated high-pressure first order specific rate k^∞ was 3.5×10^4 sec.$^{-1}$. This latter value leads to the Arrhenius-type equation, $k^\infty = 2.3 \times 10^{15}$ exp (-19.8 kcal./mole/RT) sec.$^{-1}$, for the limiting, high-pressure specific rate for an assumed activation energy equal to the dissociation energy. The frequency factor in this equation is about 100 times greater than the value (10^{13} sec.$^{-1}$) expected for a unimolecular process. If Eyring's transition state theory[10] is used as a rationale for the high value of the frequency factor, it is possible to relate this value to an entropy increase associated with the activation process. This has been done on the basis of an assumed loosely bound transition state complex in which several of the NF_2 bending vibrational modes have been weakened. The calculated frequency factor is 2×10^{15} sec.$^{-1}$ which is close to the experimental value. Carrington and Davidson[11] found this procedure useful in the interpretation of the "abnormal" frequency factor they obtained for the dissociation of N_2O_4.

4. Conclusions

Although the uncertainty in the experimental specific rate was approximately 15 percent, the dependence of the rate on total pressure indicated that the N_2F_4 dissociation reaction is unimolecular. The activation energy at 2 atm. total pressure was found to be 19.0 ± 1 kcal./mole. The high value for the Arrhenius frequency factor ($\sim 10^{15}$ sec.$^{-1}$) at the first order limit may be explained in terms of a loosely bound transition state complex.

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Chapter B-4

LITERATURE SURVEY AND ANALYSIS OF LOW-TEMPERATURE HEAT-CAPACITY DATA OF
SOME SELECTED COMPOUNDS CONTAINING
H, Li, B, N, O, F, Na, Mg, Cl, K, Br, AND I.

by George T. Furukawa and Martin L. Reilly

In the previous NBS Report 7796 (January 1, 1963) the status of the low-temperature heat-capacity data on some selected compounds of H, Li, B, N, O, F, Na, Mg, Al, Si, Cl, K, Ti, Br, and I was outlined in which the temperature range of measurements and values of S°_{298} that have been reported in the literature were summarized. The values of S°_{298} given in existing compilations were also compared.

In the present report, the results of new analyses of the existing low-temperature heat-capacity data are given on some of the above compounds. Analyses of the data on the remaining compounds will be given in the next report. Tables of thermal functions that have been calculated are given in Appendix B of this report. The values of S°_{298} obtained are compared in Table I with those reported in the original literature and by previous compilers.

As discussed in the previous NBS reports of this series, the original experimental heat-capacity data were analyzed and a table of smoothed values of heat capacity was obtained over the experimental temperature range. The values of heat capacity below the experimental range to $0^{\circ}K$ were obtained by extrapolation using the Debye heat-capacity function. Various degrees of freedom, in increasing multiples of 1.5, were applied to calculate the Debye θ from those values of heat capacity in the lower experimental temperature range. The degrees of freedom was selected that yielded the most reasonable temperature dependence of the Debye θ. The Debye θ's were extrapolated to $0^{\circ}K$ and smoothed. The values of heat capacity were calculated at each temperature from the corresponding Debye θ and the previously selected degrees of freedom. The thermal functions were evaluated from the smoothed values of heat capacity using numerical integration procedures applied to the usual thermodynamic equations.

TABLE I

Summary of Values of Entropy (S°_{298}) of Some Selected Compounds of
H, Li, B, N, O, F, Na, Mg, Cl, K, Br, and I

Chemical Formula	Gram Formula Mass	State	S°_{298}			
			This Report e.u.[b]	Original Paper e.u.[b]	References	Kelley and King (8) e.u.[b]
$LiHF_2$	45.94377	c	16.972	16.97	(14)	- - -
MgB_2	45.9340	c	8.591	8.60	(12)	8.62 ± 0.08
MgB_4	67.5560	c	12.410	12.41	(12)	12.5 ± 0.1
Na_2O_2	77.9784	c	22.694	22.6 ± 0.3	(13)	22.6 ± 0.3
NaO_2	54.9886	c	27.758	27.7 ± 0.3	(13)	27.7 ± 0.3
$NaNH_2$	39.01244	c	18.391	18.380	(4)	18.4 ± 0.2
$NaHF_2$	61.99457	c	21.719	21.73	(14)	- - -
$NaBO_2$	65.7996	c	17.573	17.574	(6)	17.57 ± 0.05
$Na_2B_4O_7$	201.2194	c	45.295	45.296	(15)	45.3 ± 0.2
		glass	44.385	44.391 ($S^\circ_{298} - S^\circ_0$)	(15)	44.4 ± 0.2 ($S^\circ_{298} - S^\circ_0$)
$KClO_3$	122.5532	c	34.184	34.17 ± 0.05	(11)	34.2 ± 0.2
$KClO_4$	138.5526	c	36.191	36.1 ± 0.3	(10)	36.1 ± 0.2
$KBrO_3$	167.0092	c	35.681	35.65	(1)	35.7 ± 0.2
KIO_3	214.0046	c	36.189	36.20	(1)	36.2 ± 0.2
$(NH_4)_2O$	52.07656	c	63.936	63.94	(7)	63.94 ± 0.10
NH_4OH	87.12251	c	39.561	39.57	(7)	39.57 ± 0.10
NH_4F	37.03698	c	17.206	17.201 ± 0.02	(3)	17.20 ± 0.05
$NH_4F \cdot H_2O$	55.05232	c	34.895	34.92	(9)	- - -
HNO_3	63.01287	1	37.213	37.19	(5)	37.19 ± 0.10
$HNO_3 \cdot H_2O$	81.02821	1	51.841	51.84	(5)	51.84 ± 0.10
$HNO_3 \cdot 3H_2O$	117.05889	1	82.897[c]	82.93[c]	(5)	82.9 ± 0.2
HgO (red)	216.5894	c	16.787	16.774	(2)	16.80 ± 0.08

[a] c = crystal, 1 = liquid g = gas
[b] e.u. = cal/deg mole
[c] The difference arises largely from the deviation of $S^\circ_{15^\circ K}$ obtained by extrapolation.

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LITERATURE SURVEY ON BERYLLIUM FLUORIDE

by K. L. Churney

A literature survey of the experimental measurements of the heat of formation of beryllium fluoride showed only two indirect determinations have been made. An analysis of these two determinations is presented in Part A. In Part B, a literature survey oriented towards the preparation and properties of BeF_2(s) is presented. The primary aim of the presentation is to assemble the significant observations made on the compound and not to discuss fluoroberyllates or phase diagrams as such. The principal conclusion is that many of the supposedly conflicting observations, the melting point of BeF_2 for example, are actually consistent with each other.

Part A. Heat of Formation of BeF_2

At the present time, the best value for the heat of formation of BeF_2(s) is based upon the measurements of Kolesov[1] for the heat of solution of the cristobalite form of BeF_2(s) and of BeO(s) in aqueous HF. His experimental results at 21°C were:

$$BeO(s) + \left[2HF + (340HF + 1300H_2O)\right] \text{ (soln)} =$$

$$\left[BeF_2 + H_2O + (340HF + 1300H_2O)\right] \text{ (soln)} - \Delta H_1; \Delta H_1 = -24.17 \pm 0.12 \text{ kcal} \quad (1)$$

$$BeF_2(s) + \left[2HF + (340HF + 1300H_2O)\right] \text{ (soln)} =$$

$$\left[BeF_2 + 2HF + (340 HF + 1300H_2O)\right] \text{ (soln)} - \Delta H_2; \Delta H_2 = -8.04 \pm 0.07 \text{ kcal} \quad (2)$$
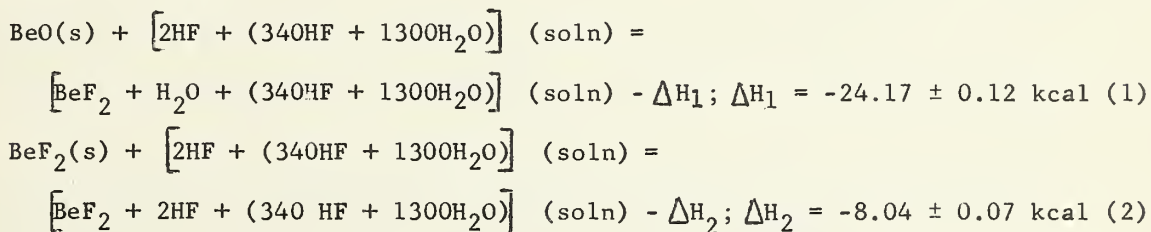
Examination of the literature showed no other measurements of the heat of solution of BeF_2(s) in aqueous HF to compare with the results in equation (2). However, other authors[2-5] have measured the heat of solution of BeO(s) in aqueous HF. As Kolesov[1] has pointed out, direct comparison of these results with equation (1) is not possible for the following reasons:
(1) Some of the authors[2-4] estimated the heat capacity of their calorimeters using an assumed or inaccurately measured heat capacity of their HF solution.
(2) Some of the samples of BeO(s) were not calcined at temperatures high enough (>1100°C.) to guarantee complete removal of the water of hydration.

In order to make a comparison, those measurements using an assumed value for the heat capacity of aqueous HF solution were corrected on the basis of the best values available at the present time[6]. An additional correction was added to convert each measurement to the change in state given by equation (1). No correction to the temperature of 21°C. was made because of lack of data and because it is probably small in comparison to other uncertainties. Uncertainties of heats of solution based upon an assumed heat capacity of aqueous HF

were estimated to be of the order of at least ± 0.5 kcal or larger, depending upon the standard deviation of the original reported values. In Table I, values for the heats of solution are presented for only those samples whose water of hydration was known, small, and allowed for in calculating the weight of BeO(s).

Table I

Heat of Solution of BeO(s) in Aqueous HF (kcal/mole BeO(s))
Corrected to the Change in State Given by Eq. (1)

Author	(5)	(3)	(3)	(4)	(5)
Date	1932	1925	1925	1925	1932
BeO(s) calcined at	390°C.	800°C.	1100°C.	(>1100°C?)	600°C.
Amount of Hydration	3 wt. %	N. R.	N. R.	N. R.	1.4 wt. %
Temperature	?	23°C.	23°C.	14°-15°, 23°C.	?
Heat of Solution					
a) Original	-24.79	-22.07	-22.21	-23.11	-24.29
Precision	±0.06[+]	±0.06[*]	±0.09[*]	±0.5[*]	±0.06[+]
b) Corrected	-24.79	-23.43	-23.66	-24.66	-24.29
Uncertainty	±0.2	±0.5	±0.5	±0.7	±0.2
Number of Measurements	5	4	3	3	5

+ Standard deviation of mean
* Average deviation   N. R. = Not Reported, value was small

Comparison of the corrected heats of solution with that given by equation (1) shows that they are in fair to good agreement. We concluded that there is at least some basis for accepting the uncertainty of Kolesov's value for the heat of solution of BeO(s) as an approximate measure of both precision and systematic error. We feel that the same is probably true for equation (2).

Of the remaining quantities required to calculate the heat of formation of BeF_2(s) from heats of solution measurements, the least certain are the heats of formation of BeO(s) and HF(g). Combustion of beryllium in oxygen has given the following results:

Table II

Author	(7)	(8)	(9)	(10)	(11)
Heat of Formation (kcal/mole)	-143.1	-147.4	-145.4	-134.1	-135.9
Uncertainty (kcal/mole)	±0.1	±0.8[*]	±0.2[*]	±0.3[*]	±1.2[*]
Number of Measurements	11	4	4	3	6

*Average deviation

The value determined by Mielenz and von Wartenberg(11) probably can be excluded on the basis of the method used to determine the heat of combustion (see (9)). Probably the result of Moose and Parr(10) should be given little weight because of the low completion of reaction (30-50%). The remaining values (7, 8, 9) are based upon heat measurements where combustion was more than 93% complete. Unfortunately, the method for the determination of the extent of combustion was not reported for the most precise value, that of Cosgrove and Snyder(7). The difference between their value and the mean of those given by Neumann, Kroger and Kunz(9) or Roth, Borger, and Siemonsen(8) suggests that Cosgrove and Snyder's value may be in error due to lack of complete combustion. The value of -143.1 ± 0.1 kcal is used in the calculation of BeF_2(s) with the understanding that it might be too positive by 2 or 3 kcal. Less accurate values for the heat of formation of BeO(s) come from heats of solution of BeO(s) and Be(s) in aqueous HF(2,12). Correction of the measurements made with Be(s) of high purity(12), using a revised heat capacity(6) for the aqueous HF solution, gives a value of -144 ± 2 to 3 kcal for the heat of formation of BeO(s).

No literature survey of the heat of formation and solution of HF(g) was made. Revised(13) values for the heat of formation of HF(g), -64.8 kcal, and heats of solution of HF(g), -10.925 kcal and H_2O(1), -0.095 kcal, in $(340HF + 1300H_2O)$ (soln) were adopted.

In order to calculate the heat of formation of BeF_2(s), equation (2) was replaced with the following equation:

$$BeF_2(s) + \left[H_2O + (340HF + 1300H_2O) \right] =$$

$$\left[BeF_2 + H_2O + (340HF + 1300H_2O) \right] - \Delta H_{2a}; \Delta H_{2a} = -8.04 \pm 0.08 \text{ kcal} \quad (2a)$$
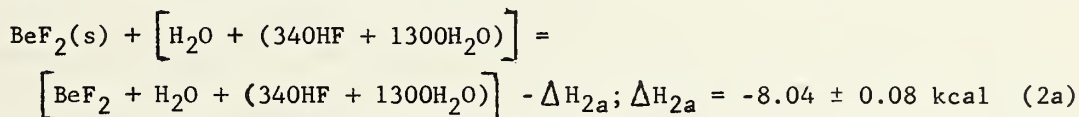
The uncertainty was increased to include the difference of equation (2a) and equation (2) (estimated to be of the order of ± 0.04 kcal).

The other equations at 298.15°K required to calculate the heat of formation of BeF_2(s) from Kolesov's measurements are (with "ss" = standard state):

$$Be(s) + 1/2 \ O_2(g,ss) = BeO(s) - \Delta H_3 \quad (3)$$

$$H_2(g,ss) + F_2(g, ss) + \left[340HF + (1300H_2O) \right] (soln) =$$

$$\left[2HF + (340HF + 1300H_2O) \right] (soln) - \Delta H_4 \quad (4)$$

$$\left[H_2O + (340HF + 1300H_2O) \right] (soln) =$$

$$H_2(g,ss) + 1/2 \ O_2(g,ss) + \left[340HF + 1300H_2O \right] (soln) - \Delta H_5 \quad (5)$$
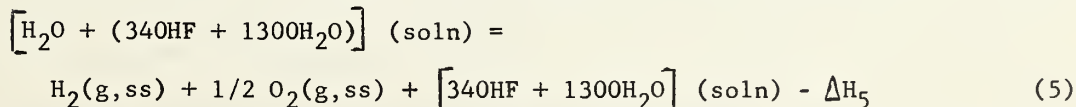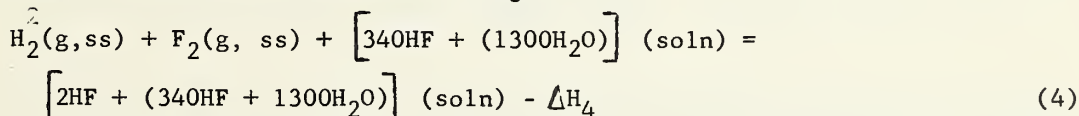
Subtracting equation (2a) from the sum of equations (1), (3), (4) and (5) gives:

$$Be(s) + F_2(g,ss) = BeF_2(s) - \Delta H_1 + \Delta H_{2a} - \Delta H_3 - \Delta H_4 - \Delta H_5 \quad (6)$$
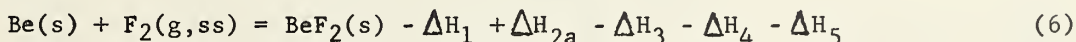
Substitution of numerical values gives:

			Precision	Systematic Error
ΔH_1		= -143.1	±0.1 kcal	(0 to -3) kcal
$-\Delta H_{2a}$		= -24.17	±0.12 kcal	
ΔH_3		= +8.04	±0.08 kcal	
$\Delta H_4 = 2[-64.8 - 10.925]$		= -151.45	±0.56 kcal	(0 to -.4) kcal
$\Delta H_5 = -[-68.317 - 0.095]$		= +68.41	±0.01 kcal	. . . . . .
		-242.27	±0.59 kcal	, (0 to -3.4) kcal

Precisions are expressed as twice the standard deviation of the mean. The precision of ΔH_4 is based upon an estimate of ±0.2 kcal uncertainty in the heat of formation of HF(g) and ±0.2 kcal uncertainty for the heat of solution of HF(g). The correction of $(\Delta H_1 - \Delta H_{2a})$ to 25°C. from 21°C. has not been included since it is small. (It is estimated to be of the order of 0.02 kcal). The systematic error of ΔH_4 is based upon the suggestion[19] made recently that a more accurate value for the heat of formation of HF(g) would be -64.93 kcal. (Their precision estimate for the heat of formation of HF(g) is ±0.15.)

The only other experimental data found in the literature survey that might be used for the determination of the heat of formation of BeF_2(s) are the measurements of Greenbaum, Arin, and Farber[14] of the equilibrium constants in the range 943-1243°K for the reaction:

$$BeO(s) + 2HF(g) = BeF_2(g) + H_2O(g) \tag{7}$$
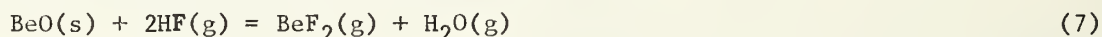
An estimate of the possible systematic error of their work was not made since we are not familiar with the field of high temperature effusion measurements. Absence of detail concerning the authors' recommended weighting procedures prevented retracing the steps of their analysis. Accordingly, the data was checked in the following approximate manner. Equilibrium constants for each of the five temperatures, where measurements were made, were weighted (assuming weighing errors alone) and averaged. These values were given equal weight. (Apriori estimates indicate this is approximate). They were combined with the thermodynamic data available in N.B.S. tables[16] and smoothed** with respect to $1/T$ as follows (i.e., using the second law method):

$$\left\{ -\ln K + \frac{1}{R}\Delta\left[-\frac{(F° - H_0°)}{T} \right] \right\} = +\frac{\Delta H_0°}{RT} - \frac{\Delta S_0°}{R} \tag{8}$$

where K is the equilibrium constant, $\Delta S_0°$ is the standard entropy change at 0°K for reaction (7). This gave values of:

$$\Delta H_0° = 24.78 \pm 3.0^* \text{ kcal} \qquad \Delta S_0° = 1.89 \pm 2.8^* \text{ cal./deg.} \tag{9}$$

$\Delta S_0°$ is found to be zero within the precision of the analysis. Hence the data are consistent with the third law. We assumed that the value obtained by Greenbaum, et al[14] for the standard heat of reaction, $\Delta H_R° = 20.5 \pm 3.4^*$,

---

**Least squares
* The uncertainty is taken as twice the standard deviation.

by smoothing lnK versus $1/T$ is the value at $1100°K$. Using the appropriate enthalpy functions(16) one obtains:

$$\Delta H_R° \; 298.15 = +23.0 \pm 3.4 \text{ kcal} \quad \text{(Greenbaum, et al)} \tag{10}$$

$$= +24.6 \pm 3.0 \text{ kcal} \quad \text{(Present Analysis)}$$

Rather than calculate the heat of formation of $BeF_2(s)$, it was suggested (18) that the heat of vaporization of $BeF_2(s)$ at $298.15°K$ be derived from a combination of Kolesov's data and equation (10) as follows:

$$BeO(s) + 2HF(g) = H_2O(g) + BeF_2(g) - \Delta H_{11} \tag{11}$$

$$BeF_2(s) + \left[H_2O + (340HF + 1300H_2O) \right] \text{ (soln)} =$$
$$\left[BeF_2 + H_2O + (340HF + 1300H_2O) \right] \text{ (soln)} - \Delta H_{12} \tag{12}$$

$$H_2O(g) + \left[340HF + 1300H_2O \right] \text{ (soln)} =$$
$$\left[H_2O + (340HF + 1300H_2O) \right] \text{ (soln)} - \Delta H_{13} \tag{13}$$

$$\left[BeF_2 + H_2O + (340HF + 1300H_2O) \right] \text{ (soln)} =$$
$$\left[2HF + (340HF + 1300H_2O) \right] \text{ (soln)} + BeO(s) - \Delta H_{14} \tag{14}$$

$$\left[2HF + (340HF + 1300H_2O) \right] \text{ (soln)} =$$
$$\left[340HF + 1300H_2O \right] \text{ (soln)} + 2HF(g) - \Delta H_{15} \tag{15}$$
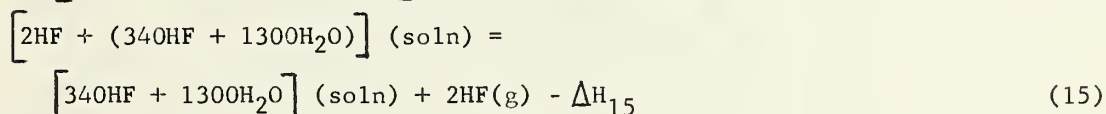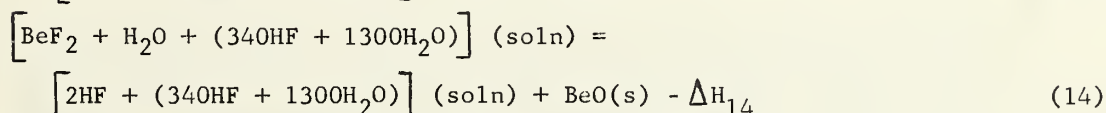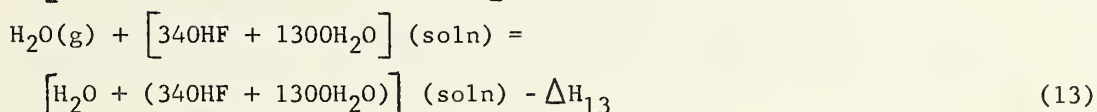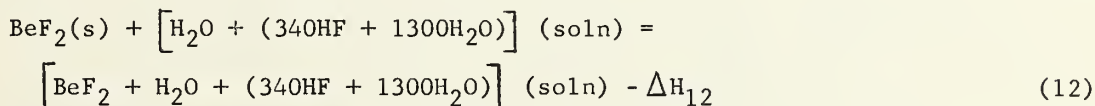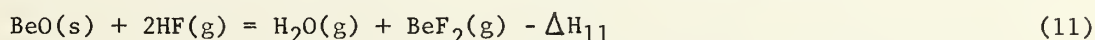
Adding equations (11) through (15) gives:

$$BeF_2(s) = BeF_2(g) - \Delta H_{16} \tag{16}$$
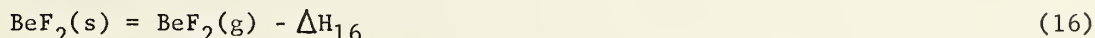
Inserting numerical values we have:

$$
\begin{array}{ll}
\Delta H_{11} & = +23.0 \pm 3.4 \text{ kcal} \\
\Delta H_{12} & = -8.04 \pm 0.08 \text{ kcal} \\
\Delta H_{13} & = -10.61 \pm 0.01 \text{ kcal} \\
\Delta H_{14} & = +24.17 \pm 0.12 \text{ kcal} \\
\Delta H_{15} = -2 \left[-10.925 \right] & = \underline{+21.85 \pm 0.28} \text{ kcal} \\
\Delta H_{16} & = +50.37 \pm 3.5 \text{ kcal}
\end{array}
$$

An independent value of the heat of vaporization of $BeF_2(s)$ at $298.15°K$ may be calculated from the thermodynamic functions of $BeF_2(g)$(16), $BeF_2(s)$(15), and the heat of vaporization of BeF_2 at $1150°K$. The latter was selected (in preference to the heat of vaporization at $0°K$.) because these thermodynamic functions of $BeF_2(s)$ are based upon the heat of vaporization of BeF_2 at $1150°K$ derived from vapor pressure measurements. The changes in state for this calculation are:

$$
\begin{array}{lll}
BeF_2(1, 1150°K) & = BeF_2(g,ss, 1150°K) - \Delta H_{17} & \tag{17} \\
BeF_2(g,ss, 1150°K) & = BeF_2(g,ss, 298.15°K) - \Delta H_{18} & \tag{18} \\
\underline{BeF_2(s, 298.15°K) = BeF_2(1, 1150°K) - \Delta H_{19}} & & \tag{19} \\
BeF_2(s, 298.15°K) & = BeF_2(g,ss, 298.15°K) - \Delta H_{20} & \tag{20}
\end{array}
$$
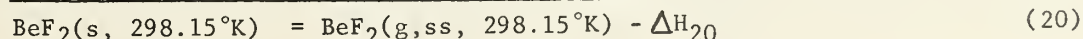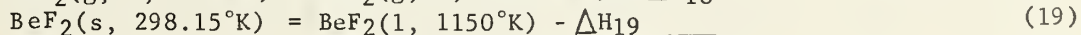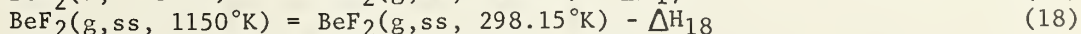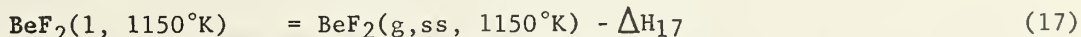
Inserting numerical values:

ΔH_{17} = 12.750 - 21.716 + 57.290 = +48.324 kcal   (15, 16)
ΔH_{18} = 2.226 - 12.750   = -10.525 kcal   (16)
ΔH_{19} = 21.716 - 1.292   = +20.424 kcal   (15)
ΔH_{20} = +58.223 kcal

Comparing the two heats of vaporization, we have:

$$\Delta H_{20} - \Delta H_{16} = 7.9 \pm 3.5 \text{ kcal}$$

This difference may be due to systematic errors in ΔH_{11} (based on Greenbaum's data), ΔH_{12} and ΔH_{14} (based on Kolesov's measurements), ΔH_{17} (the heat of vaporization of BeF_2 at 1150°K), or ΔH_{19} (based on an estimated heat capacity for $BeF_2(s)$). Our approximate analysis of Greenbaum's data suggests that different methods of treating these data will yield nearly the same result for ΔH_{11}. As indicated previously, no estimate of the systematic error in ΔH_{11} was made and the systematic errors in Kolesov's measurements, ΔH_{12} and ΔH_{14}, may be small but this is not certain. Thus, the systematic error in ΔH_{16} is unknown.

A suggestion that ΔH_{19} and hence ΔH_{20} is in error comes from another source of information. It was found in the literature survey summarized in Part B. that the heat capacity of BeF_2 has apparently been measured in the USSR (see (12), Part B.). No reference to a journal publication was found. However, in the analysis of their BeF_2 vapor pressure data, Khandamirova, et al(17) used values of $\Delta\left[-(F°-H_0°)/T\right]$ between 850-950°K for the change in state: $BeF_2(s,1) = BeF_2(g)$. These authors state that the values of $\Delta\left[-(F°-H_0°/T\right]$ are based upon "potentials for gaseous and solid BeF_2 according to the results from the Institute of Mineral Fuels and the Academy of Science of the USSR". It seems probable that the "potentials" for solid BeF_2 must be based on measured heat capacities. Assuming that their "potentials" for $BeF_2(g)$ are the same as those appearing in N.B.S. tables(16), values of $-(F°-H_0°)/T$ for $BeF_2(s)$ were calculated and are compared at three temperatures with those contained in N.B.S. tables:

Temperature	$-(F°-H_0°)/T$ for $BeF_2(s)$	
	Khandamirova(17)	N.B.S.(15)
950°K.	15.642	12.654
900°K.	14.971	11.700
850°K.	14.205	11.713

A plot of the above "potentials" versus $1/T$ gives a mean value for $(H° - H_0°)$ of $BeF_2(s)$ of 11.5 kcal from the Russian data and 16.3 kcal from the N.B.S. tables(15). This suggests that ΔH_{19} might be high by as much as 4.8 kcal.; a reduction of ΔH_{19} by 4.8 kcal would remove the discrepancy between the two heats of vaporization.

In conclusion, it should be pointed out that our analysis, although frequently speculative or only suggestive, underscores the need for measurements of the heat capacity of $BeF_2(s,1)$, a redetermination of the heat of formation of $BeO(s)$ and a direct determination of the heat of formation of $BeF_2(s)$ by combustion of $Be(s)$ in $F_2(g)$. All of these measurements are in progress, or planned for the near future, in N.B.S. laboratories.

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Part B. Crystalline Forms of BeF_2

Most of the information about the crystalline forms of BeF_2 has been derived from studies of metal fluoride - beryllium fluoride compounds and their phase relations. The "model principle"(1) and its later extension to binary systems and their phase relations (see (2), for example), although only approximate concepts(3, 4), has been a useful guide in these studies. In general, fluoroberyllates have structures that are isomorphic with the silicates although comparisons with other compounds have been made; for example, sulfates(5,6,7). The picture of BeF_2 as the approximate "weakened model" of SiO_2 is striking.

To eliminate possible confusion concerning various names given to the crystalline forms of BeF_2 in the literature, it is worthwhile noting that there are two well established forms. These are called the quartz and cristobalite forms because of their structural similarity to the forms of silica of the same name. Both forms of BeF_2 have a high and low temperature modification.

In the case of the cristobalite form, these modifications are sometimes called the hexagonal form. Another form of BeF_2, just recently reported, is called the tridymite or rhombic form of BeF_2.

BeF_2, either pure or mixed with a metal fluoride, is ordinarily prepared by thermal decomposition of $(NH_4)_2BeF_4$ (8) under reduced pressure or in a stream of CO_2 (9). Slow decomposition at temperatures less than 380°C (well under melting) in a platinum crucible yields the cristobalite form of BeF_2 (2,10,11) and in a silica crucible primarily the quartz form(12). The quartz form of BeF_2, apparently with traces of NH_4F (13), is formed when the decomposition is carried out at temperatures of 400-450°C.(14). Pure BeF_2, primarily of the quartz type, has been prepared by vacuum distillation of BeF_2 at high temperatures (800-950°C.)(12).

X-Ray examination of quenched cristobalite BeF_2 annealed at a variety of temperatures shows that slow partial conversion to the quartz form occurs between the temperatures of 430 to 516°C.(2). (504 hours were required at these two temperatures.) Below and above these temperatures only the cristobalite form is present; annealing at 542°C and above yields a glass. Heating curves of cristobalite BeF_2 show delays at 130° (small, endothermic), 400°C occasionally, 545°C. (large endothermic), and 740°C (small)(15). High temperature X-ray examination (up to 530°C.) shows apparently only one structural change--the conversion of the low temperature cristobalite form of BeF_2 to a form similar to the high-temperature cristobalite form of silica at 130°C.(15,16). Visual observation shows that the cristobalite form of BeF_2 begins to melt at 545°C. (i.e. softens); final melting occurs sluggishly in the range of 740-780°C.(11, 12,15).

The quartz form of BeF_2 was first found in a study of the NaF-BeF_2 phase diagram(11). High temp. X-ray and thermal analysis of 95 mole % BeF_2 melts in the LiF and BeF_2 phase diagram study(2,17) showed that low-temperature quartz form of BeF_2 changes reversibly at 220°C. to a form analogous to the high temperature quartz modification of silica. Heating curves of pure BeF_2 of the quartz[*] form shows delays at 220°C. (small, endothermic), ~515°C. (small), ~550°C. (large, exothermic), ~580°C (small to large, and 770°C. (small)(12). An S shaped bend in the heating curve or cooling curves, if BeF_2 is not melted, between 340-420°C. may be associated with the lambda shape in the heat capacity in this temperature range(12). X-ray examination shows apparently only the high temperature quartz form of BeF_2 between 220 and 550°C.(12). Visual examination showed that this form of BeF_2 melts completely at 545-550°C., resolidifies at about 580-590°C. and them remelts sluggishly over a broad temperature range 600-770°C. In cases where the small effect on the heating curve at 580°C. is absent the effect at 515°C. becomes large (apparently exothermic?) and a single large exothermic effect is observed at 560°C. Visual examination showed that in this case BeF_2 only melts partially at 560°C. as in the crystobalite BeF_2 study; final melting occurs at 740-770°C.[**] The last observation plus the "double" melting has prompted the suggestion that the quartz form of BeF_2 is not stable at 550°C(12, 18, 19)when it melts. Heating curves of mixtures of

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* Only a small amount of cristobalite was present.
** Melt becomes transparent.

quartz and cristobalite forms of BeF_2 (12) appear to be a superposition of those of the separate forms except for more prominent delays at 440°C. and 515°C.

Visual observations made in vapor pressure studies showed in one case the melting of BeF_2 at 545°C.(20) and in the other the presence of solid BeF_2 at ~750°C.(21); both of these are in accord with other observations. The "break" in vapor pressure curves observed by some investigators(21,22) at 800°C. has not been observed in later measurements(20,23); the possible presence of BeO(s) impurity has been offered as an explanation(24). Viscosity and electrical conductivity measurements in the interval of 700-950°C.(25) are typical of those for highly associated liquids(26) and appear to be in agreement with the observed sluggish melting of BeF_2.

Examination of phase diagram data for LiF-BeF_2(2,3,14,27,28,29) shows only the quartz form of BeF_2 is present at high BeF_2 contents (although the cristobalite form is the starting material). No thermal effects are observed above a liquidus that extrapolates to 545°C. for 100 mole % BeF_2. The proposed assignment of 337°C.(14) to a polymorphic change in BeF_2 is in doubt. Although thermal effects for the pure quartz form of BeF_2 are observed in this range, an alternative assignment to the decomposition of LiF·BeF_2 can be made. The NaF-BeF_2 phase diagram data(2,11,17,19,27,30,31) also indicates the presence of only the quartz form at high BeF_2 contents. Visual observation(19) agrees with the assignment of thermal delays observed on cooling curves in the range 650-700 and 700-750°C.(11,19) to "double melting". Heating curve delays at 425°C. for 50 mole % BeF_2 (11,19) and a group of delays above the liquidus, determined by quenching methods(2), extending to 600°C. at mole % BeF_2 (11) have been ascribed to possible "double melting"(19). In the KF-BeF_2 (27,32), MgF_2-BeF_2 (33), and PbF_2-BeF_2 (3) systems both the cristobalite and quartz forms of BeF_2 are found in devitrified mixtures at high BeF_2 contents. Devitrification near the solidus or liquidus(33,3) produces only the quartz form and at lower temperatures only the cristobalite form. The liquidus in each system extrapolates to~550°C at 100 mole % BeF_2 as does that for the NaF-BeF_2 system. In the systems RbF-BeF_2 (2,27,34), CsF-BeF_2 (35), and CaF_2-BeF_2 (33) systems only the quartz form of BeF_2 is present. The liquidus behavior at high BeF_2 content for CsF_2-BeF_2 has not been determined; those for RbF-BeF_2 and CaF_2-BeF_2 extrapolate smoothly to 545°C. High temperature X-ray examination of BeF_2 in the CsF-BeF_2 study shows that the cristobalite form is only present up to 535°C. and changes over to the quartz form which is observed up to melting, about 580°C. A related phenomena, the conversion of cristobalite to quartz form at 528°C., may have been observed in the PbF_2-BeF_2 system (33). The SrF_2-BeF_2 (36) phase diagram data suggests a eutectic with $SrBeF_4$ near 100 mole % BeF_2 with a solidus located close to the "initial" melting point (580°C.) of the quartz form which is found in devitrified melts. Thermal delays in the vicinity of 384°C. and 334°C. have tentatively been associated with those seen in this range for the pure quartz form of BeF_2. The eutectic in the BaF_2-BeF_2 (16) system also appears to lie near ~580°C. and 100 mole % BeF_2; the form of BeF_2 has not been identified. It does not appear to be either the quartz or cristobalite form. In a recent examination of the ZrF_4-BeF_2 phase diagram(37,38) another form of BeF_2 has been reported that appears when melts of high BeF_2 contents are annealed at temperatures above 550°C. to 600°C. Annealing at lower temperatures, 420-450°, yields only the quartz form. The relation of this

new form (body centered rhombic) to the cristobalite and quartz forms of BeF_2 is not certain. Because of its structural similarity to the tridymite form of SiO_2, it has been proposed to be the form of BeF_2 stable at high temperatures (18,37).

Within the limits of the literature survey, the following conclusions may be drawn:

(1) Observations made by various authors concerning the melting point of beryllium fluoride do not conflict. Greenbaum's observation(20) of a discontinuity in the vapor pressure curve at 545°C. and the appearance of glassy BeF_2 in the cooled effusion cell for runs above 545°C. offer no new information since the type of BeF_2 used was not stated. If their sample was the quartz form of BeF_2, their vapor pressure data would suggest that the observed resolidification of BeF_2 20°C. above its initial melting point is not accompanied by any appreciable exothermic effect, which is in accord with the thermal curves(12). If the sample was the cristobalite form of BeF_2, no discontinuity in the vapor pressure curve above 545°C. would be expected. Whether or not the resolidification of the quartz form above 545°C. constitutes crystallization may be questioned. The observations of Novoselova(12) suggest that this might be a change in liquid structure, although more pronounced, of the type discussed by Qurashi(39). The possibility should be examined, at least.

(2) The stable form of BeF_2 at room temperature is not known. The recent discovery of a form of BeF_2 analogous to the tridymite form of silica in a sense complicates the picture since it has been proposed that tridymite SiO_2 is not a stable crystalline phase of pure SiO_2 (40,41).

(3) The comment of Roy, Roy, and Osborn that the validity of thermal data (heating curves and cooling curves) in analyzing fusion mixtures of high BeF_2 contents is open to doubt(2) should be revised. Examination of the literature shows that heating curves yield useful information and above the liquidus curve may be the only method to obtain non-visual information.

(4) Efforts to interpret the observations by Novoselova et al (11,19) of thermal effects above the liquidus curve in the NaF-BeF_2 system as being due to the presence of impurities have not been very successful. It is possible that the thermal effects occurring for 50 mole % BeF_2 at 425°C. and extending to 600°C. at 67 mole % BeF_2 on heating curves are due to the presence of Na_2SiF_6 which decomposed in this temperature range(42). The fluorosilicate impurity would have been formed because the melts were prepared in a silica crucible. As Thilo and Budzinski have shown(43), this may lead[*] to formation of a double salt, $2Na_2BeF_4 \cdot Na_2SiF_6$, whose X-ray pattern is nearly identical to that of Na_2BeF_4. However, it is doubted if effects higher than 600°C. at higher BeF_2 contents in the NaF-BeF_2 system can be explained on this basis. Efforts to explain the latter by the presence of a BeO or $Be(OH)_2$ impurity also do not seem very fruitful since it would be expected that the former would be insoluble and the latter soluble from 545°C. to above 700°C.(see (44)).

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* Apparently, some moisture must be present.

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MASS-SPECTROMETRIC STUDY OF THE Be-O-F SYSTEM

by J. Efimenko

1. <u>Mass-Spectrometric Study of BeF$_2$</u>

Mass-spectrometric data has been obtained at NBS on the heat of sublimation of beryllium fluoride. Experimental data is presented in Table 1 and in the form of a log I$^+$ T vs ^{1}/T plot in figure 1.

Beryllium fluoride obtained by the decomposition of $(NH_4)_2BeF_4$ was supplied by the Brush Beryllium Co. A sample of this material had been ground and passed through 20 - 50 mesh. An X-ray analysis at NBS showed considerable amorphous material, 30 - 70%, and that the crystalline structure in this sample was the hexagonal form. Chemical analysis, also at NBS, indicated less than 0.01% N present. The specimen was not water-free.

The BeF$_2$ was vaporized from Mo and Ni effusion cells and figure 1 shows no trends due to container interaction. Heating was by radiation from a concentric cylindrical helix about the effusion cell. Temperature data were collected by a Pt-Pt Rh 10% thermocouple fastened into a hole in the bottom of the effusion cells. It was not possible to determine temperature gradients along the cell but no condensation was visible on the top half of the effusion cells.

It was not necessary to correct the data for fragmentation of BeF$_{2(g)}$ by the ionizing electrons because the result obtained, the heat of sublimation, was dependent on taking the differences of intensities and not absolute intensities. The log I$^+$ T vs ^{1}/T curve was fitted by least squares treatment and from the slope was obtained the average heat of sublimation ΔH°_{755} = 55.35 ± 0.53 Kcal/mol. The heat of sublimation at 0°K was computed using the data in ARPA reports nos. 6484 and 7437.

$$BeF_{2(s)} \qquad (H^{\circ}_{755} - H^{\circ}_{O})_s = 8117 \text{ cal/mol}$$

$$BeF_{2(g)} \qquad (H^{\circ}_{755} - H^{\circ}_{O})_g = 7677 \text{ cal/mol}$$

and ΔH°_{O} = 55.79 ± 0.53 Kcal/mol.

M. A. Greenbaum, J. N. Foster, M. L. Arin, and M. Farber (J. Phys. Chem. <u>67</u>, 36-40 (1963)) determined the heat of vaporization for liquid BeF$_2$. They obtained a value ΔH°_{1000} = 53.22 ± 0.18 Kcal/mol from a log p vs ^{1}/T plot. Correcting their value to 755°K one obtains 53.8 ± 0.3 Kcal/mol. The data from the above experiments cannot serve to determine the heat of fusion of beryllium fluoride because the errors affecting the accuracy of the two methods may not cancel.

2. BeO - BeF$_2$ System

Some preliminary and tentative experimental information from NBS work is presented for the BeO-BeF$_2$ system.

On reacting the two compounds in an effusion cell, the intensity of mass 72 rises with temperature. No similar intensity-temperature change is observed at this mass position with BeO or BeF$_2$ alone. The specie corresponding to that mass (72) responds to a shutter interposed in the effusing beam and indicates that it originates in the reaction cell containing BeO and BeF$_2$. Since Be and F have only one isotope each and the isotopes O^{17} and O^{18} cannot be detected, isotope ratio checks cannot be made. However, the evidence obtained suggests that probability is large that mass 72 corresponds to the complex molecule Be$_2$OF$_2$.

From the ion intensities of masses 47 and 72 the heat of formation of the complex molecules was obtained. The tentative value of this heat of formation has an estimated error of ±15 Kcal/mole which arises from some experimental difficulties. Further work is in progress to improve the thermodynamic data.

Table 1

DATA

$$BeF_2 \; \rightleftarrows \; BeF_2 \, (g)$$
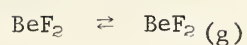
Index No.	T, °K	I^+ (1 volt)	$I^+ T$	$10^3 / T$
1	721	1.60	1153	1.3870
2	723	1.60	1157	1.3831
3	724	1.70	1232	1.3812
4	749.1	6.00	4495	1.3349
5	749.7	6.40	4798	1.3339
6	754.4	7.50	5658	1.3256
7	780.3	24.3	18960	1.2816
8	780.1	24.3	18960	1.2819
9	783.2	27.3	21380	1.2768
10	781.1	26.1	20390	1.2802
11	781	24.9	19450	1.2804
12	780	24.3	18950	1.2821
13	795.1	47.0	37370	1.2577
14	796	48.0	38210	1.2563
15	796.5	50.0	39830	1.2555
16	778	23.0	17890	1.2853
17	778	23.3	18130	1.2853
18	777.5	22.8	17730	1.2862
19	776	20.1	15600	1.2887
20	753.5	6.90	5199	1.3271
21	753	6.75	5083	1.3280
22	714	0.95	678	1.4006
23	714	0.90	643	1.4006
24	745.5	4.80	3578	1.3414
25	745.7	4.75	3542	1.3410
26	747.1	5.10	3810	1.3385
27	748.8	6.40	4792	1.3355
28	786.0	29.5	23190	1.2723
29	785.4	29.0	22780	1.2732
30	818.9	111.0	90900	1.2212
31	790.1	38.0	30020	1.2657
32	789.1	38.0	29990	1.2673

Index No.	T, °K	I^+ (1 volt)	$I^+ T$	$10^3 / T$
33	787.9	38.0	29940	1.2692
34	785.5	34.2	26860	1.2731
35	762.2	12.8	9756	1.3119
36	768	13.5	10370	1.3021
37	768	13.8	10600	1.3021
38	767	13.8	10580	1.3038
39	767	13.5	10350	1.3038
40	777	21.5	16710	1.2870
41	738	3.65	2694	1.3550
42	735	3.45	2536	1.3605
43	705	0.66	465	1.4184
44	710	0.80	568	1.4085
45	746	5.15	3842	1.3405
46	737	3.35	2469	1.3569
47	730	2.75	2008	1.3699
48	776	23.7	18390	1.2887
49	772	19.8	15290	1.2953
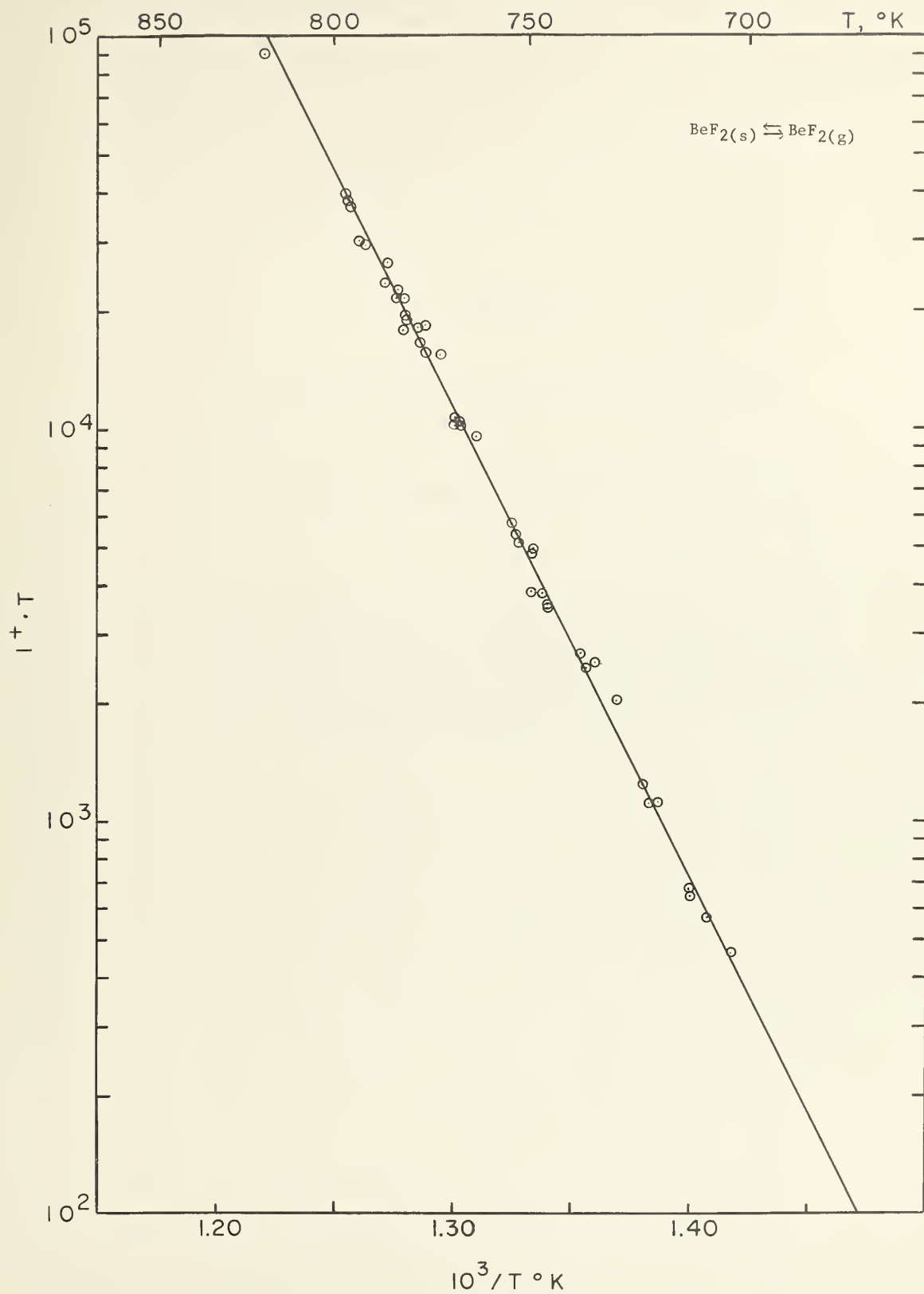
FIGURE 1

The curve is a least squares fit to the data of Table I. The heat of sublimation
obtained from this curve is 55.35 ± 0.53 Kcal/mol for the average temperature, 755°K.

APPENDIX B

THERMODYNAMIC FUNCTIONS OF SOLIDS AND LIQUIDS

by

George T. Furukawa and Martin L. Reilly

The calculation of these tables is discussed in chapter B-4 of this report. The tables form a supplement to similar tables in Appendix B of earlier reports and the numbering of these tables is continuous with the earlier ones. No table of this report replaces or duplicates a table of any previous report.

THERMODYNAMIC FUNCTIONS FOR LITHIUM MONOHYDROGEN DIFLUORIDE (LI H F$_2$)
SOLID PHASE

GRAM MOLECULAR WT.=45.94377 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	0.000	0.001	0.001	0.004	0.003	0.001
10.00	0.002	0.007	0.009	0.068	0.027	0.023
15.00	0.007	0.021	0.029	0.317	0.078	0.112
20.00	0.017	0.045	0.062	0.904	0.164	0.332
25.00	0.030	0.082	0.112	2.046	0.303	0.759
30.00	0.050	0.135	0.185	4.046	0.509	1.490
35.00	0.076	0.208	0.283	7.269	0.793	2.648
40.00	0.109	0.302	0.412	12.096	1.149	4.373
45.00	0.151	0.419	0.570	18.852	1.562	6.816
50.00	0.203	0.556	0.759	27.802	2.024	10.127
55.00	0.263	0.712	0.975	39.151	2.520	14.448
60.00	0.332	0.884	1.216	53.040	3.040	19.914
65.00	0.410	1.071	1.480	69.586	3.579	26.646
70.00	0.496	1.269	1.765	88.815	4.112	34.753
75.00	0.591	1.476	2.067	110.69	4.639	44.327
80.00	0.693	1.690	2.383	135.21	5.168	55.446
85.00	0.802	1.910	2.712	162.36	5.692	68.180
90.00	0.918	2.134	3.052	192.09	6.196	82.586
95.00	1.039	2.361	3.400	224.29	6.680	98.713
100.00	1.166	2.589	3.755	258.85	7.142	116.60
105.00	1.298	2.816	4.114	295.67	7.583	136.27
110.00	1.434	3.043	4.477	334.68	8.019	157.74
115.00	1.574	3.268	4.842	375.84	8.443	181.04
120.00	1.718	3.492	5.210	419.07	8.843	206.17
125.00	1.865	3.714	5.579	464.24	9.226	233.14
130.00	2.015	3.933	5.948	511.30	9.595	261.96
135.00	2.168	4.149	6.317	560.16	9.947	292.62
140.00	2.322	4.362	6.685	610.75	10.285	325.13
145.00	2.479	4.572	7.051	662.99	10.610	359.47
150.00	2.638	4.779	7.416	716.83	10.921	395.64
155.00	2.798	4.982	7.779	772.18	11.219	433.63
160.00	2.959	5.181	8.140	829.00	11.505	473.43
165.00	3.121	5.377	8.498	887.22	11.780	515.03
170.00	3.285	5.569	8.854	946.78	12.045	558.41
175.00	3.449	5.758	9.207	1007.7	12.303	603.56
180.00	3.614	5.943	9.557	1069.8	12.553	650.47
185.00	3.779	6.125	9.904	1133.2	12.798	699.13
190.00	3.945	6.304	10.249	1197.8	13.036	749.51
195.00	4.111	6.480	10.590	1263.5	13.267	801.61
200.00	4.277	6.652	10.929	1330.4	13.491	855.41
205.00	4.443	6.822	11.265	1398.4	13.706	910.90
210.00	4.610	6.988	11.598	1467.5	13.912	968.06
215.00	4.776	7.151	11.927	1537.5	14.109	1026.9
220.00	4.942	7.312	12.254	1608.5	14.298	1087.3
225.00	5.108	7.469	12.577	1680.5	14.480	1149.4
230.00	5.274	7.623	12.898	1753.3	14.655	1213.1
235.00	5.440	7.775	13.214	1827.0	14.824	1278.4
240.00	5.605	7.923	13.528	1901.6	14.989	1345.2
245.00	5.770	8.069	13.839	1976.9	15.151	1413.7
250.00	5.934	8.212	14.147	2053.1	15.311	1483.6
255.00	6.098	8.353	14.452	2130.0	15.470	1555.1
260.00	6.262	8.491	14.753	2207.8	15.628	1628.1
265.00	6.425	8.628	15.053	2286.3	15.785	1702.6
270.00	6.588	8.762	15.349	2365.6	15.941	1778.7
273.15	6.690	8.845	15.535	2416.0	16.039	1827.3
275.00	6.750	8.893	15.643	2445.7	16.096	1856.1
280.00	6.911	9.023	15.934	2526.6	16.248	1935.1
285.00	7.072	9.152	16.223	2608.2	16.398	2015.5
290.00	7.232	9.278	16.510	2690.6	16.547	2097.3
295.00	7.392	9.402	16.794	2773.7	16.695	2180.6
298.15	7.492	9.480	16.972	2826.4	16.787	2233.8
300.00	7.551	9.525	17.076	2857.5	16.841	2265.2

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

TABLE B-85

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM DIBORIDE (MG B$_2$)
SOLID PHASE

GRAM MOLECULAR WT.=45.9340 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	0.000	0.000	0.000	0.000	0.000	0.000
10.00	0.000	0.000	0.001	0.004	0.002	0.001
15.00	0.000	0.001	0.002	0.021	0.005	0.007
20.00	0.001	0.003	0.004	0.060	0.011	0.022
25.00	0.002	0.006	0.008	0.153	0.031	0.051
30.00	0.004	0.013	0.017	0.385	0.060	0.111
35.00	0.006	0.022	0.028	0.771	0.101	0.221
40.00	0.010	0.035	0.045	1.409	0.153	0.403
45.00	0.015	0.052	0.067	2.350	0.234	0.682
50.00	0.022	0.076	0.098	3.820	0.354	1.092
55.00	0.031	0.107	0.138	5.892	0.478	1.679
60.00	0.041	0.144	0.186	8.652	0.630	2.483
65.00	0.055	0.189	0.243	12.271	0.830	3.551
70.00	0.071	0.244	0.314	17.062	1.088	4.939
75.00	0.090	0.308	0.398	23.116	1.332	6.715
80.00	0.112	0.381	0.492	30.449	1.605	8.935
85.00	0.137	0.460	0.597	39.115	1.854	11.656
90.00	0.166	0.545	0.710	49.010	2.112	14.921
95.00	0.198	0.634	0.832	60.261	2.383	18.774
100.00	0.233	0.728	0.960	72.794	2.632	23.252
105.00	0.270	0.825	1.096	86.669	2.929	28.389
110.00	0.311	0.928	1.239	102.07	3.220	34.224
115.00	0.355	1.033	1.388	118.80	3.477	40.789
120.00	0.401	1.142	1.543	137.02	3.831	48.111
125.00	0.450	1.255	1.705	156.89	4.113	56.228
130.00	0.501	1.371	1.872	178.22	4.422	65.168
135.00	0.555	1.490	2.045	201.11	4.733	74.959
140.00	0.612	1.611	2.223	225.53	5.035	85.626
145.00	0.670	1.734	2.405	251.47	5.341	97.192
150.00	0.731	1.859	2.591	278.92	5.638	109.68
155.00	0.794	1.986	2.780	307.83	5.925	123.10
160.00	0.859	2.113	2.973	338.16	6.203	137.49
165.00	0.926	2.241	3.168	369.85	6.470	152.84
170.00	0.995	2.370	3.365	402.85	6.730	169.17
175.00	1.066	2.498	3.564	437.14	6.985	186.49
180.00	1.138	2.626	3.764	472.70	7.236	204.81
185.00	1.212	2.754	3.966	509.50	7.485	224.13
190.00	1.287	2.882	4.168	547.54	7.732	244.46
195.00	1.363	3.009	4.372	586.82	7.976	265.82
200.00	1.441	3.137	4.577	627.30	8.218	288.19
205.00	1.520	3.263	4.783	668.99	8.455	311.59
210.00	1.600	3.390	4.990	711.84	8.687	336.02
215.00	1.681	3.516	5.197	755.85	8.914	361.49
220.00	1.764	3.641	5.404	800.97	9.134	387.99
225.00	1.847	3.765	5.612	847.18	9.346	415.54
230.00	1.931	3.889	5.820	894.42	9.550	444.11
235.00	2.016	4.011	6.027	942.66	9.746	473.73
240.00	2.102	4.133	6.234	991.86	9.936	504.39
245.00	2.188	4.253	6.441	1042.0	10.121	536.08
250.00	2.275	4.372	6.647	1093.1	10.304	568.80
255.00	2.363	4.490	6.853	1145.0	10.484	602.55
260.00	2.451	4.607	7.059	1197.9	10.659	637.33
265.00	2.540	4.723	7.263	1251.6	10.829	673.13
270.00	2.629	4.838	7.467	1306.2	10.988	709.96
273.15	2.686	4.909	7.595	1340.9	11.082	733.68
275.00	2.719	4.951	7.670	1361.5	11.134	747.80
280.00	2.809	5.062	7.872	1417.5	11.265	786.66
285.00	2.900	5.172	8.072	1474.1	11.379	826.52
290.00	2.991	5.280	8.271	1531.2	11.476	867.38
295.00	3.082	5.386	8.468	1588.8	11.554	909.23
298.15	3.140	5.451	8.591	1625.3	11.594	936.10
300.00	3.174	5.489	8.663	1646.8	11.613	952.06

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

TABLE B-86

THERMODYNAMIC FUNCTIONS FOR MAGNESIUM TETRABORIDE (MG B_4)
SOLID PHASE

GRAM MOLECULAR WT.=67.5560 GRAMS   1 CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^0)/T$ $\dfrac{CAL}{DEG\ MOLE}$	$(H_T^0-H_0^0)/T$ $\dfrac{CAL}{DEG\ MOLE}$	$(S_T^0-S_0^0)$ $\dfrac{CAL}{DEG\ MOLE}$	$(H_T^0-H_0^0)$ $\dfrac{CAL}{MOLE}$	C_P^0 $\dfrac{CAL}{DEG\ MOLE}$	$-(G_T^0-H_0^0)$ $\dfrac{CAL}{MOLE}$
0.00	0.000	0.000	0.000	0.000	0.000	0.000
10.00	0.000	0.001	0.001	0.011	0.004	0.004
15.00	0.001	0.004	0.005	0.055	0.014	0.019
20.00	0.003	0.008	0.011	0.158	0.027	0.057
25.00	0.005	0.014	0.019	0.357	0.063	0.130
30.00	0.009	0.035	0.044	1.049	0.244	0.277
35.00	0.018	0.078	0.096	2.726	0.405	0.620
40.00	0.031	0.127	0.158	5.068	0.538	1.250
45.00	0.049	0.183	0.233	8.246	0.756	2.219
50.00	0.072	0.255	0.327	12.763	1.046	3.611
55.00	0.100	0.339	0.439	18.651	1.315	5.522
60.00	0.134	0.432	0.566	25.940	1.591	8.031
65.00	0.172	0.530	0.702	34.452	1.813	11.199
70.00	0.215	0.632	0.847	44.210	2.115	15.067
75.00	0.263	0.743	1.005	55.718	2.482	19.692
80.00	0.314	0.862	1.176	68.960	2.817	25.142
85.00	0.370	0.987	1.357	83.897	3.155	31.471
90.00	0.430	1.117	1.547	100.49	3.485	38.729
95.00	0.494	1.250	1.744	118.74	3.811	46.953
100.00	0.562	1.386	1.947	138.55	4.109	56.180
105.00	0.633	1.522	2.155	159.82	4.401	66.434
110.00	0.707	1.660	2.366	182.58	4.704	77.735
115.00	0.784	1.799	2.583	206.91	5.036	90.106
120.00	0.863	1.942	2.805	232.99	5.398	103.57
125.00	0.945	2.087	3.032	260.83	5.738	118.16
130.00	1.030	2.234	3.264	290.42	6.096	133.90
135.00	1.117	2.384	3.501	321.79	6.453	150.81
140.00	1.207	2.535	3.742	354.95	6.809	168.91
145.00	1.298	2.689	3.987	389.88	7.164	188.23
150.00	1.392	2.844	4.236	426.57	7.513	208.79
155.00	1.488	3.000	4.488	464.99	7.855	230.60
160.00	1.585	3.157	4.742	505.11	8.190	253.67
165.00	1.685	3.314	4.999	546.89	8.522	278.02
170.00	1.786	3.473	5.259	590.33	8.856	303.67
175.00	1.889	3.631	5.520	635.46	9.196	330.62
180.00	1.994	3.791	5.784	682.31	9.548	358.88
185.00	2.100	3.951	6.051	730.95	9.910	388.46
190.00	2.207	4.113	6.320	781.42	10.277	419.39
195.00	2.316	4.275	6.592	833.72	10.641	451.67
200.00	2.427	4.439	6.866	887.81	10.996	485.31
205.00	2.538	4.603	7.141	943.65	11.338	520.33
210.00	2.651	4.767	7.419	1001.2	11.667	556.73
215.00	2.765	4.932	7.697	1060.3	11.989	594.52
220.00	2.880	5.096	7.976	1121.1	12.308	633.70
225.00	2.997	5.260	8.256	1183.4	12.631	674.28
230.00	3.114	5.423	8.538	1247.4	12.957	716.26
235.00	3.233	5.587	8.820	1313.0	13.282	759.66
240.00	3.352	5.751	9.103	1380.2	13.603	804.46
245.00	3.472	5.914	9.386	1449.0	13.916	850.68
250.00	3.593	6.077	9.671	1519.3	14.220	898.33
255.00	3.715	6.240	9.955	1591.2	14.517	947.39
260.00	3.838	6.402	10.240	1664.5	14.809	997.88
265.00	3.961	6.563	10.525	1739.3	15.100	1049.8
270.00	4.086	6.724	10.810	1815.5	15.390	1103.1
273.15	4.164	6.825	10.989	1864.3	15.572	1137.5
275.00	4.210	6.884	11.095	1893.2	15.678	1157.9
280.00	4.336	7.044	11.380	1972.3	15.957	1214.1
285.00	4.462	7.202	11.665	2052.7	16.221	1271.7
290.00	4.589	7.360	11.949	2134.4	16.460	1330.7
295.00	4.716	7.516	12.232	2217.2	16.667	1391.2
298.15	4.796	7.613	12.410	2269.9	16.778	1430.0
300.00	4.843	7.670	12.514	2301.0	16.835	1453.0

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

TABLE B-87

THERMODYNAMIC FUNCTIONS FOR SODIUM PEROXIDE (NA$_2$O$_2$)
SOLID PHASE

GRAM MOLECULAR WT.=77.9784 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	0.000	0.001	0.001	0.005	0.004	0.002
10.00	0.002	0.007	0.010	0.073	0.029	0.024
15.00	0.008	0.024	0.033	0.367	0.098	0.122
20.00	0.019	0.058	0.077	1.160	0.232	0.387
25.00	0.038	0.113	0.151	2.820	0.446	0.944
30.00	0.065	0.192	0.257	5.763	0.744	1.948
35.00	0.102	0.297	0.399	10.389	1.119	3.573
40.00	0.150	0.427	0.577	17.092	1.576	5.998
45.00	0.209	0.584	0.793	26.298	2.118	9.409
50.00	0.280	0.765	1.045	38.254	2.649	13.993
55.00	0.362	0.960	1.322	52.786	3.190	19.898
60.00	0.454	1.175	1.629	70.483	3.910	27.260
65.00	0.558	1.415	1.972	91.959	4.682	36.249
70.00	0.672	1.675	2.347	117.28	5.441	47.037
75.00	0.797	1.951	2.748	146.35	6.186	59.766
80.00	0.932	2.239	3.171	179.15	6.935	74.555
85.00	1.077	2.537	3.614	215.67	7.671	91.511
90.00	1.230	2.842	4.073	255.82	8.384	110.72
95.00	1.392	3.152	4.545	299.47	9.075	132.26
100.00	1.562	3.465	5.027	346.49	9.727	156.18
105.00	1.738	3.778	5.517	396.70	10.353	182.54
110.00	1.921	4.091	6.012	450.01	10.971	211.36
115.00	2.110	4.403	6.513	506.38	11.569	242.67
120.00	2.304	4.714	7.018	565.64	12.131	276.50
125.00	2.503	5.021	7.524	627.64	12.663	312.85
130.00	2.706	5.325	8.031	692.23	13.169	351.74
135.00	2.912	5.624	8.537	759.28	13.647	393.16
140.00	3.122	5.919	9.041	828.66	14.100	437.10
145.00	3.335	6.209	9.544	900.24	14.530	483.57
150.00	3.550	6.493	10.043	973.92	14.938	532.53
155.00	3.768	6.772	10.539	1049.6	15.326	583.99
160.00	3.987	7.045	11.032	1127.1	15.694	637.92
165.00	4.208	7.312	11.520	1206.5	16.044	694.30
170.00	4.430	7.574	12.004	1287.6	16.376	753.11
175.00	4.653	7.830	12.483	1370.2	16.689	814.33
180.00	4.877	8.080	12.957	1454.4	16.985	877.94
185.00	5.102	8.325	13.427	1540.0	17.265	943.90
190.00	5.327	8.563	13.891	1627.0	17.531	1012.2
195.00	5.553	8.797	14.349	1715.3	17.786	1082.8
200.00	5.778	9.024	14.803	1804.9	18.031	1155.7
205.00	6.004	9.247	15.251	1895.6	18.267	1230.8
210.00	6.229	9.464	15.694	1987.5	18.495	1308.2
215.00	6.455	9.677	16.132	2080.6	18.713	1387.7
220.00	6.679	9.885	16.564	2174.6	18.919	1469.5
225.00	6.904	10.088	16.992	2269.7	19.114	1553.4
230.00	7.128	10.286	17.414	2365.8	19.298	1639.4
235.00	7.351	10.480	17.831	2462.7	19.473	1727.5
240.00	7.574	10.669	18.242	2560.5	19.642	1817.7
245.00	7.796	10.854	18.649	2659.1	19.809	1909.9
250.00	8.017	11.034	19.051	2758.6	19.975	2004.2
255.00	8.237	11.211	19.448	2858.9	20.139	2100.4
260.00	8.456	11.384	19.841	2960.0	20.300	2198.6
265.00	8.675	11.554	20.229	3061.8	20.457	2298.8
270.00	8.892	11.720	20.613	3164.5	20.607	2400.9
273.15	9.029	11.823	20.852	3229.6	20.698	2466.2
275.00	9.109	11.883	20.992	3267.9	20.750	2504.9
280.00	9.324	12.043	21.367	3372.0	20.886	2610.8
285.00	9.539	12.199	21.738	3476.8	21.017	2718.6
290.00	9.752	12.352	22.105	3582.2	21.148	2828.2
295.00	9.965	12.502	22.467	3688.2	21.279	2939.7
298.15	10.098	12.596	22.694	3755.4	21.363	3010.8
300.00	10.176	12.650	22.826	3795.0	21.414	3052.9

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

THERMODYNAMIC FUNCTIONS FOR SODIUM SUPEROXIDE (NA O$_2$)
SOLID PHASES

GRAM MOLECULAR WT.=54.9886 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	0.001	0.003	0.004	0.014	0.011	0.005
10.00	0.007	0.022	0.029	0.217	0.087	0.072
15.00	0.024	0.073	0.097	1.094	0.289	0.366
20.00	0.057	0.169	0.227	3.385	0.655	1.147
25.00	0.110	0.316	0.425	7.888	1.167	2.748
30.00	0.184	0.507	0.691	15.203	1.771	5.512
35.00	·0.279	0.734	1.013	25.699	2.439	9.749
40.00	0.393	0.993	1.386	39.722	3.186	15.725
45.00	0.527	1.282	1.809	57.710	4.013	23.693
50.00	0.678	1.589	2.266	79.444	4.605	33.876
55.00	0.843	1.882	2.724	103.49	5.058	46.353
60.00	1.019	2.176	3.195	130.57	5.801	61.142
65.00	1.205	2.485	3.691	161.54	6.583	78.347
70.00	1.401	2.805	4.206	196.35	7.330	98.082
75.00	1.606	3.130	4.736	234.73	8.014	120.43
80.00	1.818	3.455	5.273	276.36	8.623	145.45
85.00	2.037	3.775	5.812	320.88	9.183	173.16
90.00	2.262	4.092	6.354	368.25	9.771	203.58
95.00	2.492	4.406	6.898	418.57	10.348	236.70
100.00	2.726	4.716	7.442	471.64	10.874	272.55
105.00	2.963	5.022	7.985	527.27	11.377	311.12
110.00	3.204	5.322	8.525	585.40	11.875	352.39
115.00	3.447	5.617	9.064	645.98	12.350	396.37
120.00	3.692	5.907	9.599	708.83	12.783	443.03
125.00	3.939	6.191	10.130	773.85	13.220	492.35
130.00	4.187	6.469	10.656	840.98	13.630	544.32
135.00	4.436	6.742	11.178	910.12	14.022	598.90
140.00	4.686	7.008	11.695	981.17	14.394	656.09
145.00	4.937	7.269	12.206	1054.0	14.739	715.84
150.00	5.188	7.523	12.711	1128.5	15.057	778.15
155.00	5.438	7.771	13.209	1204.5	15.343	842.95
160.00	5.689	8.012	13.701	1281.9	15.598	910.23
165.00	5.939	8.245	14.184	1360.4	15.820	979.95
170.00	6.189	8.471	14.659	1440.0	16.014	1052.1
175.00	6.437	8.689	15.126	1520.5	16.182	1126.5
180.00	6.685	8.899	15.584	1601.8	16.328	1203.3
185.00	6.932	9.102	16.033	1683.8	16.456*	1282.4
190.00	7.177	9.297	16.474	1766.3	16.568*	1363.6
195.00	7.421	9.484	16.905	1849.4	16.666*	1447.1
196.20	7.479	9.528	17.008	1869.5	16.688*	1467.4
196.20	7.479	11.431	18.910	2242.8	16.688*	1467.4
200.00	7.699	11.531	19.231	2306.3	16.752*	1539.9
205.00	7.986	11.660	19.645	2390.2	16.827*	1637.1
210.00	8.268	11.784	20.052	2474.5	16.893*	1736.3
215.00	8.547	11.903	20.450	2559.2	16.950*	1837.6
220.00	8.822	12.018	20.840	2644.0	16.999*	1940.8
221.70	8.915	12.057	20.971	2672.9	17.014*	1976.4
221.70	8.915	13.757	22.671	3049.8	17.014*	1976.4
225.00	9.118	13.805	22.923	3106.0	17.042*	2051.6
230.00	9.422	13.875	23.298	3191.3	17.079*	2167.1
235.00	9.722	13.944	23.665	3276.8	17.110*	2284.6
240.00	10.016	14.010	24.026	3362.4	17.137	2403.8
245.00	10.305	14.074	24.380	3448.2	17.159	2524.8
250.00	10.590	14.136	24.726	3534.0	17.177	2647.6
255.00	10.871	14.196	25.067	3619.9	17.190	2772.1
260.00	11.147	14.254	25.401	3705.9	17.199	2898.2
265.00	11.419	14.309	25.728	3791.9	17.205	3026.0
270.00	11.687	14.363	26.050	3878.0	17.209	3155.5
273.15	11.854	14.396	26.249	3932.2	17.211	3237.9
275.00	11.951	14.415	26.366	3964.0	17.212	3286.5
280.00	12.211	14.465	26.676	4050.1	17.214	3419.1
285.00	12.468	14.513	26.980	4136.2	17.219	3553.3
290.00	12.720	14.560	27.280	4222.3	17.225	3688.9
295.00	12.970	14.605	27.575	4308.4	17.235	3826.1
298.15	13.125	14.633	27.758	4362.7	17.244	3913.2
300.00	13.216	14.649	27.864	4394.6	17.250	3964.7

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

* HYPOTHETICAL HEAT CAPACITIES IN THE RANGE OF THE TRANSITIONS

TABLE B-89

THERMODYNAMIC FUNCTIONS FOR SODIUM AMIDE (NA N H$_2$)
SOLID PHASE

GRAM MOLECULAR WT.=39.01244 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	0.000	0.000	0.001	0.002	0.002	0.001
10.00	0.002	0.007	0.008	0.067	0.038	0.016
15.00	0.010	0.047	0.057	0.703	0.259	0.151
20.00	0.036	0.148	0.184	2.952	0.656	0.720
25.00	0.084	0.291	0.375	7.281	1.067	2.096
30.00	0.151	0.452	0.603	13.571	1.447	4.530
35.00	0.233	0.623	0.856	21.790	1.861	8.169
40.00	0.329	0.810	1.138	32.384	2.371	13.141
45.00	0.435	1.004	1.439	45.194	2.736	19.582
50.00	0.551	1.197	1.748	59.861	3.151	27.546
55.00	0.674	1.397	2.072	76.857	3.658	37.089
60.00	0.805	1.606	2.411	96.376	4.126	48.291
65.00	0.942	1.816	2.758	118.04	4.553	61.210
70.00	1.084	2.029	3.113	142.02	5.035	75.883
75.00	1.231	2.244	3.476	168.34	5.490	92.352
80.00	1.383	2.462	3.845	196.93	5.948	110.65
85.00	1.539	2.680	4.219	227.83	6.413	130.81
90.00	1.698	2.900	4.598	261.01	6.853	152.85
95.00	1.861	3.119	4.980	296.32	7.266	176.80
100.00	2.027	3.336	5.363	333.62	7.649	202.65
105.00	2.195	3.550	5.745	372.76	8.006	230.42
110.00	2.365	3.761	6.126	413.73	8.383	260.10
115.00	2.536	3.970	6.507	456.59	8.758	291.68
120.00	2.710	4.177	6.887	501.25	9.098	325.17
125.00	2.884	4.381	7.265	547.60	9.441	360.55
130.00	3.060	4.582	7.642	595.62	9.765	397.81
135.00	3.237	4.779	8.016	645.22	10.075	436.96
140.00	3.414	4.974	8.388	696.35	10.375	477.97
145.00	3.592	5.165	8.757	748.94	10.659	520.84
150.00	3.770	5.353	9.123	802.93	10.933	565.54
155.00	3.949	5.537	9.486	858.25	11.195	612.06
160.00	4.127	5.718	9.845	914.86	11.448	660.39
165.00	4.306	5.895	10.201	972.72	11.692	710.51
170.00	4.485	6.069	10.554	1031.8	11.928	762.40
175.00	4.663	6.240	10.903	1092.0	12.157	816.04
180.00	4.841	6.407	11.249	1153.3	12.379	871.42
185.00	5.019	6.572	11.591	1215.8	12.592	928.52
190.00	5.196	6.733	11.929	1279.2	12.796	987.32
195.00	5.373	6.891	12.264	1343.7	12.990	1047.8
200.00	5.550	7.046	12.595	1409.1	13.173	1110.0
205.00	5.726	7.197	12.923	1475.4	13.347	1173.8
210.00	5.901	7.346	13.246	1542.6	13.512	1239.2
215.00	6.075	7.491	13.566	1610.5	13.672	1306.2
220.00	6.249	7.633	13.882	1679.3	13.828	1374.8
225.00	6.422	7.773	14.195	1748.8	13.981	1445.0
230.00	6.595	7.909	14.504	1819.1	14.133	1516.8
235.00	6.766	8.043	14.809	1890.1	14.281	1590.1
240.00	6.937	8.175	15.112	1961.9	14.426	1664.9
245.00	7.107	8.304	15.410	2034.4	14.565	1741.2
250.00	7.276	8.430	15.706	2107.5	14.699	1819.0
255.00	7.444	8.554	15.998	2181.4	14.826	1898.2
260.00	7.611	8.676	16.287	2255.8	14.948	1978.9
265.00	7.778	8.796	16.573	2330.8	15.063	2061.1
270.00	7.943	8.913	16.856	2406.4	15.174	2144.7
273.15	8.047	8.985	17.032	2454.3	15.243	2198.0
275.00	8.108	9.028	17.135	2482.6	15.282	2229.7
280.00	8.272	9.140	17.412	2559.2	15.390	2316.0
285.00	8.434	9.251	17.685	2636.5	15.498	2403.8
290.00	8.596	9.359	17.956	2714.2	15.610	2492.9
295.00	8.757	9.466	18.223	2792.6	15.728	2583.3
298.15	8.858	9.533	18.391	2842.2	15.806	2641.0
300.00	8.917	9.572	18.489	2871.5	15.854	2675.1

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

TABLE B-90

THERMODYNAMIC FUNCTIONS FOR SODIUM MONOHYDROGEN DIFLUORIDE (NA H F$_2$)
SOLID PHASE

GRAM MOLECULAR WT.=61.99457 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	0.001	0.002	0.003	0.010	0.008	0.003
10.00	0.005	0.016	0.021	0.159	0.063	0.054
15.00	0.018	0.053	0.070	0.788	0.206	0.268
20.00	0.041	0.120	0.161	2.394	0.456	0.827
25.00	0.078	0.221	0.300	5.536	0.819	1.959
30.00	0.130	0.358	0.489	10.748	1.282	3.909
35.00	0.198	0.529	0.727	18.532	1.848	6.928
40.00	0.282	0.733	1.015	29.336	2.479	11.265
45.00	0.381	0.964	1.345	43.376	3.144	17.148
50.00	0.496	1.217	1.712	60.845	3.847	24.777
55.00	0.624	1.488	2.113	81.860	4.558	34.327
60.00	0.766	1.774	2.539	106.41	5.263	45.947
65.00	0.919	2.069	2.988	134.47	5.954	59.757
70.00	1.084	2.370	3.454	165.89	6.610	75.855
75.00	1.257	2.674	3.931	200.52	7.237	94.312
80.00	1.440	2.977	4.417	238.20	7.827	115.18
85.00	1.629	3.279	4.909	278.75	8.392	138.49
90.00	1.825	3.579	5.404	322.07	8.929	164.27
95.00	2.027	3.873	5.900	367.95	9.414	192.53
100.00	2.233	4.161	6.394	416.14	9.859	223.27
105.00	2.443	4.443	6.886	466.51	10.284	256.47
110.00	2.656	4.718	7.373	518.94	10.684	292.12
115.00	2.871	4.985	7.857	573.31	11.059	330.20
120.00	3.089	5.246	8.335	629.48	11.404	370.68
125.00	3.308	5.499	8.807	687.35	11.741	413.53
130.00	3.529	5.745	9.274	746.85	12.057	458.74
135.00	3.750	5.984	9.735	807.90	12.359	506.26
140.00	3.972	6.217	10.189	870.42	12.646	556.07
145.00	4.194	6.444	10.638	934.33	12.914	608.14
150.00	4.416	6.663	11.080	999.52	13.156	662.44
155.00	4.638	6.876	11.515	1065.8	13.365	718.93
160.00	4.860	7.082	11.943	1133.2	13.589	777.67
165.00	5.081	7.283	12.364	1201.7	13.803	838.44
170.00	5.302	7.478	12.779	1271.2	14.007	901.31
175.00	5.521	7.667	13.188	1341.7	14.203	966.23
180.00	5.740	7.851	13.591	1413.2	14.391	1033.2
185.00	5.957	8.030	13.988	1485.6	14.573	1102.1
190.00	6.174	8.205	14.379	1558.9	14.749	1173.0
195.00	6.389	8.375	14.764	1633.1	14.920	1245.9
200.00	6.603	8.541	15.144	1708.1	15.087	1320.7
205.00	6.816	8.702	15.519	1784.0	15.250	1397.3
210.00	7.028	8.860	15.888	1860.6	15.410	1475.9
215.00	7.238	9.014	16.252	1938.1	15.566	1556.2
220.00	7.447	9.165	16.612	2016.3	15.721	1638.4
225.00	7.655	9.312	16.967	2095.3	15.873	1722.3
230.00	7.861	9.457	17.318	2175.0	16.023	1808.0
235.00	8.066	9.598	17.664	2255.5	16.171	1895.5
240.00	8.269	9.736	18.006	2336.7	16.318	1984.7
245.00	8.472	9.872	18.344	2418.7	16.464	2075.5
250.00	8.672	10.005	18.678	2501.4	16.609	2168.1
255.00	8.872	10.136	19.008	2584.8	16.752	2262.3
260.00	9.070	10.265	19.335	2668.9	16.894	2358.2
265.00	9.267	10.391	19.658	2753.7	17.036	2455.7
270.00	9.462	10.516	19.978	2839.2	17.177	2554.7
273.15	9.584	10.593	20.177	2893.5	17.265	2618.0
275.00	9.656	10.638	20.294	2925.5	17.317	2655.4
280.00	9.849	10.759	20.607	3012.4	17.456	2757.7
285.00	10.040	10.877	20.918	3100.0	17.595	2861.5
290.00	10.231	10.994	21.225	3188.4	17.733	2966.9
295.00	10.419	11.110	21.529	3277.4	17.871	3073.7
298.15	10.538	11.182	21.719	3333.8	17.957	3141.9
300.00	10.607	11.224	21.831	3367.1	18.008	3182.1

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

THERMODYNAMIC FUNCTIONS FOR SODIUM METABORATE (NA B O_2)
SOLID PHASE

GRAM MOLECULAR WT.=65.7996 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	$\frac{CAL}{DEG\ MOLE}$	$\frac{CAL}{DEG\ MOLE}$	$\frac{CAL}{DEG\ MOLE}$	$\frac{CAL}{MOLE}$	$\frac{CAL}{DEG\ MOLE}$	$\frac{CAL}{MOLE}$
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	0.001
10.00	0.002	0.005	0.007	0.051	0.023	0.016
15.00	0.006	0.021	0.027	0.311	0.090	0.092
20.00	0.016	0.054	0.070	1.076	0.232	0.322
25.00	0.034	0.112	0.146	2.806	0.478	0.846
30.00	0.062	0.201	0.263	6.035	0.830	1.851
35.00	0.101	0.322	0.423	11.266	1.276	3.548
40.00	0.154	0.473	0.626	18.904	1.788	6.155
45.00	0.219	0.649	0.869	29.210	2.340	9.877
50.00	0.298	0.847	1.145	42.341	2.914	14.898
55.00	0.389	1.061	1.449	58.350	3.488	21.372
60.00	0.491	1.287	1.777	77.211	4.054	29.431
65.00	0.603	1.521	2.124	98.869	4.604	39.191
70.00	0.724	1.760	2.484	123.21	5.127	50.707
75.00	0.854	2.001	2.855	150.10	5.625	64.053
80.00	0.991	2.243	3.234	179.42	6.098	79.273
85.00	1.134	2.483	3.617	211.04	6.547	96.397
90.00	1.283	2.720	4.003	244.84	6.971	115.45
95.00	1.436	2.955	4.391	280.71	7.371	136.43
100.00	1.594	3.185	4.779	318.52	7.749	159.36
105.00	1.754	3.411	5.166	358.16	8.107	184.22
110.00	1.918	3.632	5.551	399.55	8.446	211.01
115.00	2.085	3.849	5.933	442.60	8.768	239.72
120.00	2.253	4.060	6.313	487.21	9.076	270.34
125.00	2.423	4.267	6.689	533.33	9.370	302.84
130.00	2.594	4.468	7.062	580.89	9.653	337.22
135.00	2.766	4.666	7.432	629.84	9.925	373.46
140.00	2.940	4.858	7.798	680.13	10.187	411.54
145.00	3.113	5.046	8.160	731.70	10.440	451.43
150.00	3.288	5.230	8.518	784.51	10.684	493.13
155.00	3.462	5.410	8.872	838.53	10.920	536.60
160.00	3.636	5.586	9.222	893.70	11.149	581.84
165.00	3.811	5.758	9.569	950.00	11.370	628.81
170.00	3.985	5.926	9.911	1007.4	11.585	677.52
175.00	4.160	6.091	10.250	1065.8	11.794	727.92
180.00	4.333	6.252	10.585	1125.3	11.997	780.01
185.00	4.507	6.410	10.917	1185.8	12.194	833.77
190.00	4.680	6.564	11.244	1247.3	12.386	889.17
195.00	4.852	6.716	11.569	1309.7	12.574	946.20
200.00	5.024	6.865	11.889	1373.0	12.757	1004.8
205.00	5.196	7.011	12.206	1437.2	12.936	1065.1
210.00	5.366	7.154	12.520	1502.3	13.111	1126.9
215.00	5.536	7.295	12.831	1568.3	13.283	1190.3
220.00	5.705	7.433	13.138	1635.2	13.451	1255.2
225.00	5.874	7.568	13.442	1702.8	13.616	1321.7
230.00	6.042	7.701	13.743	1771.3	13.778	1389.6
235.00	6.209	7.832	14.041	1840.6	13.937	1459.1
240.00	6.375	7.961	14.336	1910.7	14.094	1530.0
245.00	6.541	8.088	14.629	1981.5	14.248	1602.4
250.00	6.705	8.213	14.918	2053.2	14.399	1676.3
255.00	6.869	8.335	15.205	2125.5	14.549	1751.6
260.00	7.032	8.456	15.488	2198.6	14.696	1828.4
265.00	7.194	8.575	15.770	2272.5	14.841	1906.5
270.00	7.356	8.693	16.049	2347.0	14.985	1986.0
273.15	7.457	8.766	16.223	2394.4	15.075	2036.9
275.00	7.516	8.808	16.325	2422.3	15.127	2067.0
280.00	7.676	8.923	16.599	2498.3	15.267	2149.3
285.00	7.835	9.035	16.870	2575.0	15.405	2233.0
290.00	7.993	9.146	17.139	2652.4	15.542	2318.0
295.00	8.150	9.256	17.406	2730.4	15.677	2404.4
298.15	8.249	9.324	17.573	2779.9	15.761	2459.4
300.00	8.307	9.364	17.671	2809.1	15.811	2492.0

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

TABLE B-92

THERMODYNAMIC FUNCTIONS FOR CRYSTALLINE SODIUM TETRABORATE ($NA_2B_4O_7$)
SOLID PHASE

GRAM MOLECULAR WT.=201.2194 GRAMS   , CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0-H^0_0)/T$ CAL DEG⁻MOLE	$(H^0-H^0_0)/T$ CAL DEG⁻MOLE	$(S^0-S^0_0)$ CAL DEG⁻MOLE	$(H^0-H^0_0)$ CAL MOLE	C^0_P CAL DEG⁻MOLE	$-(G^0-H^0_0)$ CAL MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.002	0.003	0.012	0.009	0.004
10.00	0.006	0.018	0.025	0.185	0.080	0.060
15.00	0.023	0.080	0.103	1.202	0.378	0.343
20.00	0.063	0.221	0.284	4.412	0.949	1.264
25.00	0.135	0.446	0.581	11.142	1.777	3.375
30.00	0.242	0.747	0.989	22.420	2.756	7.257
35.00	0.384	1.112	1.496	38.919	3.861	13.431
40.00	0.559	1.528	2.087	61.135	5.053	22.356
45.00	0.765	1.985	2.749	89.306	6.239	34.421
50.00	0.999	2.471	3.470	123.55	7.460	49.948
55.00	1.258	2.980	4.238	163.88	8.670	69.200
60.00	1.540	3.504	5.044	210.24	9.869	92.390
65.00	1.841	4.039	5.881	262.55	11.049	119.69
70.00	2.161	4.580	6.741	320.63	12.176	151.24
75.00	2.495	5.123	7.618	384.24	13.265	187.13
80.00	2.843	5.666	8.509	453.28	14.352	227.44
85.00	3.203	6.209	9.411	527.73	15.420	272.24
90.00	3.573	6.749	10.322	607.38	16.429	321.57
95.00	3.952	7.283	11.235	691.90	17.370	375.46
100.00	4.339	7.810	12.150	781.04	18.286	433.92
105.00	4.733	8.331	13.064	874.75	19.192	496.95
110.00	5.132	8.845	13.977	972.92	20.073	564.56
115.00	5.537	9.352	14.888	1075.4	20.933	636.72
120.00	5.945	9.852	15.797	1182.2	21.783	713.44
125.00	6.358	10.346	16.703	1293.2	22.617	794.69
130.00	6.773	10.834	17.607	1408.4	23.434	880.47
135.00	7.191	11.315	18.506	1527.6	24.234	970.75
140.00	7.611	11.791	19.402	1650.7	25.017	1065.5
145.00	8.033	12.260	20.293	1777.7	25.784	1164.8
150.00	8.456	12.723	21.180	1908.5	26.535	1268.4
155.00	8.881	13.181	22.062	2043.0	27.272	1376.5
160.00	9.307	13.633	22.939	2181.2	27.997	1489.1
165.00	9.733	14.079	23.812	2323.0	28.709	1605.9
170.00	10.160	14.519	24.679	2468.3	29.409	1727.2
175.00	10.587	14.955	25.541	2617.1	30.098	1852.7
180.00	11.014	15.385	26.399	2769.2	30.776	1982.6
185.00	11.442	15.810	27.251	2924.8	31.445	2116.7
190.00	11.869	16.230	28.099	3083.7	32.106	2255.1
195.00	12.296	16.645	28.941	3245.8	32.760	2397.7
200.00	12.722	17.056	29.779	3411.3	33.407	2544.5
205.00	13.149	17.463	30.611	3579.9	34.047	2695.4
210.00	13.574	17.865	31.440	3751.7	34.681	2850.6
215.00	13.999	18.264	32.263	3926.7	35.307	3009.8
220.00	14.424	18.658	33.082	4104.8	35.923	3173.2
225.00	14.847	19.049	33.896	4285.9	36.531	3340.6
230.00	15.270	19.435	34.705	4470.1	37.128	3512.2
235.00	15.692	19.818	35.510	4657.2	37.717	3687.7
240.00	16.114	20.197	36.310	4847.2	38.299	3867.2
245.00	16.534	20.572	37.106	5040.2	38.874	4050.8
250.00	16.953	20.944	37.897	5236.0	39.443	4238.3
255.00	17.372	21.312	38.684	5434.6	40.008	4429.7
260.00	17.789	21.677	39.466	5636.0	40.567	4625.1
265.00	18.205	22.039	40.244	5840.2	41.119	4824.4
270.00	18.621	22.397	41.018	6047.2	41.665	5027.6
273.15	18.882	22.621	41.503	6179.0	42.005	5157.5
275.00	19.035	22.752	41.787	6256.9	42.204	5234.6
280.00	19.448	23.104	42.552	6469.2	42.736	5445.4
285.00	19.860	23.453	43.313	6684.2	43.262	5660.1
290.00	20.271	23.799	44.070	6901.8	43.784	5878.5
295.00	20.681	24.143	44.823	7122.1	44.302	6100.8
298.15	20.938	24.357	45.295	7262.1	44.628	6242.7
300.00	21.089	24.483	45.572	7344.9	44.819	6326.8

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

TABLE B-93

THERMODYNAMIC FUNCTIONS FOR VITREOUS SODIUM TETRABORATE ($NA_2B_4O_7$)
SOLID PHASE

GRAM MOLECULAR WT.=201.2194 GRAMS   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	0.001	0.003	0.004	0.015	0.012	0.005
10.00	0.008	0.027	0.036	0.273	0.122	0.084
15.00	0.033	0.111	0.144	1.665	0.484	0.490
20.00	0.085	0.276	0.362	5.524	1.091	1.707
25.00	0.171	0.514	0.685	12.844	1.865	4.281
30.00	0.291	0.815	1.105	24.445	2.800	8.718
35.00	0.442	1.171	1.614	40.998	3.836	15.482
40.00	0.625	1.573	2.197	62.908	4.936	24.981
45.00	0.835	2.009	2.844	90.413	6.070	37.560
50.00	1.070	2.473	3.543	123.63	7.220	53.506
55.00	1.328	2.957	4.285	162.61	8.369	73.059
60.00	1.607	3.455	5.062	207.30	9.504	96.413
65.00	1.903	3.963	5.867	257.61	10.614	123.72
70.00	2.216	4.477	6.693	313.40	11.697	155.12
75.00	2.542	4.994	7.536	374.53	12.751	190.68
80.00	2.881	5.511	8.392	440.86	13.777	230.50
85.00	3.231	6.026	9.257	512.25	14.775	274.62
90.00	3.590	6.540	10.129	588.56	15.746	323.08
95.00	3.957	7.049	11.006	669.66	16.689	375.92
100.00	4.331	7.554	11.886	755.41	17.606	433.15
105.00	4.712	8.054	12.766	845.69	18.500	494.78
110.00	5.098	8.549	13.647	940.37	19.372	560.81
115.00	5.489	9.038	14.527	1039.4	20.225	631.25
120.00	5.884	9.522	15.406	1142.6	21.061	706.08
125.00	6.282	10.000	16.282	1250.0	21.883	785.30
130.00	6.684	10.472	17.156	1361.4	22.690	868.90
135.00	7.088	10.940	18.027	1476.8	23.485	956.86
140.00	7.494	11.402	18.896	1596.2	24.268	1049.2
145.00	7.902	11.859	19.761	1719.5	25.038	1145.8
150.00	8.312	12.311	20.622	1846.6	25.798	1246.8
155.00	8.723	12.758	21.481	1977.5	26.546	1352.0
160.00	9.135	13.200	22.335	2112.0	27.284	1461.6
165.00	9.548	13.638	23.186	2250.3	28.011	1575.4
170.00	9.961	14.071	24.033	2392.1	28.728	1693.4
175.00	10.375	14.500	24.876	2537.5	29.435	1815.7
180.00	10.790	14.925	25.715	2686.5	30.133	1942.2
185.00	11.205	15.345	26.550	2838.9	30.822	2072.8
190.00	11.619	15.761	27.381	2994.7	31.503	2207.7
195.00	12.034	16.174	28.208	3153.9	32.174	2346.6
200.00	12.449	16.582	29.031	3316.4	32.838	2489.7
205.00	12.863	16.987	29.850	3482.2	33.494	2636.9
210.00	13.277	17.387	30.665	3651.3	34.142	2788.2
215.00	13.691	17.784	31.475	3823.6	34.782	2943.6
220.00	14.104	18.178	32.282	3999.1	35.415	3103.0
225.00	14.517	18.568	33.085	4177.8	36.040	3266.4
230.00	14.930	18.954	33.884	4359.5	36.658	3433.8
235.00	15.341	19.338	34.679	4544.3	37.269	3605.2
240.00	15.753	19.718	35.470	4732.2	37.873	3780.6
245.00	16.163	20.094	36.257	4923.1	38.469	3959.9
250.00	16.573	20.468	37.040	5116.9	39.059	4143.2
255.00	16.982	20.838	37.819	5313.6	39.642	4330.3
260.00	17.390	21.205	38.595	5513.3	40.217	4521.4
265.00	17.797	21.569	39.366	5715.8	40.786	4716.3
270.00	18.204	21.930	40.134	5921.1	41.348	4916.0
273.15	18.459	22.156	40.616	6051.9	41.698	5042.2
275.00	18.609	22.288	40.898	6129.3	41.903	5117.6
280.00	19.014	22.643	41.658	6340.2	42.452	5324.0
285.00	19.418	22.996	42.414	6553.8	42.994	5534.2
290.00	19.821	23.345	43.166	6770.1	43.529	5748.1
295.00	20.223	23.692	43.915	6989.1	44.058	5965.8
298.15	20.476	23.909	44.385	7128.4	44.388	6104.9
300.00	20.624	24.036	44.660	7210.7	44.581	6187.3

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

TABLE B-94

THERMODYNAMIC FUNCTIONS FOR POTASSIUM CHLORATE (K CL O$_3$)
SOLID PHASE

GRAM MOLECULAR WT.=122.5532 GRAMS   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	0.006	0.008	0.031	0.025	0.010
10.00	0.016	0.048	0.064	0.481	0.187	0.163
15.00	0.053	0.155	0.208	2.326	0.620	0.798
20.00	0.125	0.379	0.505	7.589	1.552	2.503
25.00	0.245	0.726	0.971	18.156	2.721	6.128
30.00	0.416	1.173	1.588	35.181	4.073	12.471
35.00	0.634	1.672	2.306	58.532	5.262	22.177
40.00	0.891	2.199	3.090	87.955	6.513	35.641
45.00	1.181	2.745	3.927	123.53	7.693	53.165
50.00	1.499	3.293	4.793	164.67	8.749	74.954
55.00	1.838	3.835	5.673	210.90	9.726	101.11
60.00	2.195	4.363	6.558	261.76	10.604	131.69
65.00	2.564	4.874	7.438	316.82	11.402	166.68
70.00	2.944	5.366	8.309	375.59	12.088	206.06
75.00	3.330	5.834	9.164	437.57	12.693	249.75
80.00	3.721	6.281	10.002	502.46	13.264	297.67
85.00	4.115	6.708	10.823	570.18	13.813	349.74
90.00	4.510	7.116	11.626	640.44	14.277	405.87
95.00	4.905	7.504	12.409	712.87	14.686	465.96
100.00	5.299	7.872	13.171	787.20	15.045	529.92
105.00	5.692	8.222	13.914	863.35	15.419	597.64
110.00	6.082	8.558	14.640	941.38	15.787	669.03
115.00	6.470	8.879	15.349	1021.1	16.098	744.01
120.00	6.854	9.186	16.040	1102.3	16.375	822.49
125.00	7.235	9.479	16.714	1184.9	16.665	904.39
130.00	7.612	9.761	17.373	1268.9	16.932	989.61
135.00	7.986	10.031	18.017	1354.2	17.196	1078.1
140.00	8.355	10.292	18.647	1440.0	17.457	1169.8
145.00	8.721	10.543	19.264	1528.8	17.711	1264.5
150.00	9.083	10.786	19.869	1618.0	17.962	1362.4
155.00	9.440	11.022	20.462	1708.4	18.208	1463.2
160.00	9.794	11.250	21.044	1800.0	18.450	1567.0
165.00	10.143	11.472	21.615	1892.9	18.689	1673.6
170.00	10.489	11.688	22.177	1986.9	18.927	1783.1
175.00	10.831	11.898	22.729	2082.2	19.165	1895.4
180.00	11.169	12.103	23.272	2178.6	19.404	2010.4
185.00	11.503	12.304	23.807	2276.2	19.640	2128.1
190.00	11.834	12.500	24.334	2375.0	19.872	2248.5
195.00	12.161	12.692	24.853	2474.9	20.097	2371.4
200.00	12.485	12.880	25.364	2575.9	20.312	2497.0
205.00	12.805	13.063	25.869	2678.0	20.519	2625.1
210.00	13.122	13.243	26.365	2781.1	20.719	2755.6
215.00	13.436	13.419	26.855	2885.2	20.915	2888.7
220.00	13.746	13.592	27.338	2990.2	21.110	3024.2
225.00	14.054	13.761	27.815	3096.3	21.307	3162.1
230.00	14.358	13.927	28.285	3203.3	21.508	3302.3
235.00	14.659	14.091	28.750	3311.4	21.714	3444.9
240.00	14.958	14.252	29.209	3420.5	21.922	3589.8
245.00	15.253	14.411	29.664	3530.6	22.129	3737.0
250.00	15.546	14.567	30.113	3641.7	22.330	3886.4
255.00	15.836	14.721	30.557	3753.9	22.519	4038.1
260.00	16.123	14.873	30.996	3866.9	22.692	4192.0
265.00	16.408	15.022	31.430	3980.8	22.847	4348.1
270.00	16.690	15.168	31.858	4095.4	22.988	4506.3
273.15	16.866	15.259	32.125	4167.9	23.073	4607.1
275.00	16.970	15.311	32.281	4210.6	23.124	4666.6
280.00	17.247	15.452	32.699	4326.6	23.269	4829.1
285.00	17.521	15.591	33.112	4443.4	23.441	4993.6
290.00	17.794	15.728	33.522	4561.1	23.659	5160.2
295.00	18.064	15.865	33.928	4680.1	23.941	5328.8
298.15	18.233	15.951	34.184	4755.8	24.160	5436.1
300.00	18.332	16.002	34.334	4800.6	24.305	5499.5

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

TABLE B-95

THERMODYNAMIC FUNCTIONS FOR POTASSIUM PERCHLORATE (K CL O$_4$)
SOLID PHASE

GRAM MOLECULAR WT.=138.5526 GRAMS   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	0.003	0.008	0.011	0.040	0.032	0.013
10.00	0.022	0.068	0.089	0.676	0.286	0.217
15.00	0.078	0.244	0.322	3.653	0.944	1.171
20.00	0.183	0.515	0.699	10.305	1.779	3.668
25.00	0.336	0.888	1.225	22.206	3.021	8.409
30.00	0.538	1.357	1.895	40.698	4.397	16.155
35.00	0.787	1.894	2.681	66.289	5.831	27.554
40.00	1.078	2.470	3.548	98.811	7.152	43.101
45.00	1.402	3.057	4.459	137.56	8.326	63.106
50.00	1.755	3.638	5.392	181.88	9.384	87.729
55.00	2.128	4.204	6.332	231.22	10.334	117.04
60.00	2.517	4.751	7.268	285.04	11.176	151.04
65.00	2.918	5.273	8.191	342.73	11.859	189.70
70.00	3.327	5.766	9.093	403.61	12.585	232.92
75.00	3.742	6.259	10.001	469.45	13.697	280.65
80.00	4.161	6.736	10.898	538.91	13.962	332.91
85.00	4.583	7.167	11.750	609.22	14.250	389.54
90.00	5.004	7.575	12.579	681.75	14.744	450.38
95.00	5.424	7.963	13.387	756.46	15.134	515.30
100.00	5.842	8.330	14.173	833.04	15.485	584.21
105.00	6.257	8.678	14.935	911.22	15.793	656.99
110.00	6.668	9.011	15.679	991.19	16.209	733.53
115.00	7.076	9.333	16.409	1073.3	16.608	813.76
120.00	7.480	9.643	17.123	1157.2	16.966	897.59
125.00	7.880	9.942	17.822	1242.8	17.263	984.96
130.00	8.275	10.229	18.505	1329.8	17.551	1075.8
135.00	8.667	10.506	19.172	1418.3	17.821	1170.0
140.00	9.053	10.772	19.825	1508.0	18.086	1267.5
145.00	9.436	11.028	20.464	1599.1	18.356	1368.2
150.00	9.814	11.277	21.091	1691.6	18.629	1472.1
155.00	10.188	11.519	21.707	1785.4	18.906	1579.1
160.00	10.557	11.754	22.311	1880.6	19.183	1689.2
165.00	10.922	11.983	22.906	1977.2	19.453	1802.2
170.00	11.283	12.207	23.490	2075.2	19.715	1918.2
175.00	11.640	12.425	24.065	2174.4	19.968	2037.1
180.00	11.994	12.638	24.631	2274.8	20.216	2158.8
185.00	12.343	12.846	25.189	2376.5	20.465	2283.4
190.00	12.688	13.050	25.738	2479.5	20.721	2410.7
195.00	13.029	13.250	26.280	2583.8	20.987	2540.8
200.00	13.367	13.447	26.814	2689.4	21.260	2673.5
205.00	13.702	13.641	27.343	2796.4	21.536	2808.9
210.00	14.033	13.832	27.865	2904.7	21.804	2946.9
215.00	14.361	14.020	28.381	3014.4	22.056	3087.5
220.00	14.685	14.206	28.891	3125.2	22.288	3230.7
225.00	15.006	14.388	29.394	3237.2	22.499	3376.4
230.00	15.324	14.566	29.891	3350.2	22.696	3524.6
235.00	15.640	14.741	30.381	3464.2	22.892	3675.3
240.00	15.952	14.913	30.865	3579.1	23.097	3828.4
245.00	16.261	15.082	31.343	3695.2	23.320	3984.0
250.00	16.567	15.250	31.817	3812.4	23.563	4141.9
255.00	16.871	15.415	32.286	3930.8	23.825	4302.1
260.00	17.172	15.579	32.751	4050.6	24.096	4464.7
265.00	17.470	15.743	33.213	4171.8	24.368	4629.6
270.00	17.766	15.905	33.671	4294.3	24.636	4796.8
273.15	17.951	16.006	33.958	4372.2	24.802	4903.3
275.00	18.059	16.066	34.125	4418.1	24.899	4966.3
280.00	18.350	16.226	34.576	4543.3	25.163	5138.1
285.00	18.639	16.385	35.024	4669.8	25.441	5312.1
290.00	18.925	16.544	35.469	4797.8	25.748	5488.3
295.00	19.209	16.703	35.912	4927.3	26.097	5666.8
298.15	19.387	16.803	36.191	5009.9	26.344	5780.3
300.00	19.491	16.863	36.354	5058.8	26.500	5847.4

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

TABLE B-96

THERMODYNAMIC FUNCTIONS FOR POTASSIUM BROMATE (K Br O$_3$)
SOLID PHASE

GRAM MOLECULAR WT.=167.0092 GRAMS   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^{-1}MOLE^{-1}	CAL DEG^{-1}MOLE^{-1}	CAL DEG^{-1}MOLE^{-1}	CAL MOLE^{-1}	CAL DEG^{-1}MOLE^{-1}	CAL MOLE^{-1}
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.002	0.007	0.009	0.035	0.028	0.012
10.00	0.019	0.057	0.076	0.568	0.228	0.189
15.00	0.064	0.192	0.256	2.876	0.761	0.959
20.00	0.150	0.437	0.587	8.744	1.629	3.002
25.00	0.283	0.782	1.065	19.559	2.741	7.075
30.00	0.463	1.218	1.681	36.541	4.071	13.886
35.00	0.688	1.721	2.409	60.233	5.387	24.073
40.00	0.952	2.255	3.207	90.188	6.576	38.090
45.00	1.249	2.798	4.047	125.89	7.701	56.210
50.00	1.572	3.343	4.916	167.17	8.804	78.605
55.00	1.916	3.887	5.803	213.78	9.816	105.40
60.00	2.277	4.419	6.696	265.13	10.711	136.65
65.00	2.652	4.935	7.587	320.78	11.538	172.35
70.00	3.036	5.433	8.469	380.33	12.262	212.50
75.00	3.427	5.910	9.337	443.27	12.907	257.02
80.00	3.823	6.367	10.191	509.39	13.540	305.85
85.00	4.222	6.806	11.028	578.51	14.085	358.90
90.00	4.623	7.223	11.847	650.10	14.547	416.10
95.00	5.025	7.621	12.646	724.01	15.018	477.33
100.00	5.425	8.003	13.428	800.28	15.491	542.53
105.00	5.825	8.371	14.195	878.91	15.960	611.59
110.00	6.222	8.726	14.948	959.86	16.414	684.45
115.00	6.618	9.069	15.687	1043.0	16.828	761.05
120.00	7.011	9.401	16.412	1128.1	17.222	841.30
125.00	7.401	9.721	17.122	1215.1	17.573	925.14
130.00	7.768	10.029	17.818	1303.8	17.911	1012.5
135.00	8.173	10.327	18.500	1394.2	18.236	1103.3
140.00	8.553	10.615	19.169	1486.2	18.551	1197.5
145.00	8.931	10.894	19.825	1579.7	18.860	1295.0
150.00	9.305	11.165	20.470	1674.7	19.161	1395.7
155.00	9.675	11.428	21.103	1771.3	19.455	1499.6
160.00	10.042	11.683	21.725	1869.3	19.739	1606.7
165.00	10.405	11.931	22.337	1968.7	20.016	1716.9
170.00	10.765	12.173	22.938	2069.4	20.285	1830.3
175.00	11.121	12.409	23.530	2171.5	20.548	1946.2
180.00	11.474	12.638	24.112	2274.9	20.804	2065.3
185.00	11.824	12.862	24.686	2379.5	21.054	2187.3
190.00	12.169	13.081	25.251	2485.4	21.295	2312.2
195.00	12.512	13.295	25.807	2592.5	21.526	2439.8
200.00	12.851	13.503	26.354	2700.6	21.744	2570.2
205.00	13.187	13.707	26.894	2809.9	21.948	2703.4
210.00	13.520	13.905	27.425	2920.1	22.140	2839.2
215.00	13.849	14.099	27.948	3031.3	22.321	2977.6
220.00	14.176	14.288	28.463	3143.3	22.494	3118.6
225.00	14.499	14.472	28.971	3256.2	22.662	3262.2
230.00	14.819	14.652	29.471	3369.9	22.828	3408.3
235.00	15.136	14.828	29.963	3484.5	22.993	3556.9
240.00	15.450	14.999	30.449	3599.9	23.160	3708.0
245.00	15.761	15.168	30.929	3716.1	23.328	3861.4
250.00	16.069	15.333	31.402	3833.1	23.498	4017.2
255.00	16.374	15.494	31.868	3951.1	23.669	4175.4
260.00	16.677	15.653	32.330	4069.8	23.841	4335.9
265.00	16.976	15.809	32.786	4189.5	24.015	4498.7
270.00	17.273	15.963	33.236	4310.0	24.189	4663.8
273.15	17.459	16.058	33.517	4386.4	24.299	4768.9
275.00	17.567	16.114	33.682	4431.4	24.363	4831.1
280.00	17.859	16.263	34.122	4553.6	24.534	5000.6
285.00	18.148	16.409	34.558	4676.7	24.700	5172.3
290.00	18.435	16.554	34.989	4800.6	24.859	5346.1
295.00	18.719	16.696	35.415	4925.3	25.009	5522.1
298.15	18.897	16.784	35.681	5004.2	25.097	5634.1
300.00	19.001	16.836	35.836	5050.7	25.147	5700.3

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

TABLE B-97

THERMODYNAMIC FUNCTIONS FOR POTASSIUM IODATE (K I O$_3$)
SOLID PHASE

GRAM MOLECULAR WT.=214.0046 GRAMS   CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T	$-(G_T^0-H_0^0)/T$	$(H_T^0-H_0^0)/T$	$(S_T^0-S_C^0)$	$(H_T^0-H_0^0)$	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	0.003	0.008	0.010	0.038	0.031	0.013
10.00	0.020	0.061	0.082	0.612	0.245	0.204
15.00	0.069	0.206	0.275	3.089	0.817	1.032
20.00	0.161	0.470	0.632	9.409	1.752	3.229
25.00	0.304	0.837	1.141	20.925	2.892	7.603
30.00	0.495	1.286	1.781	38.575	4.165	14.860
35.00	0.731	1.785	2.515	62.466	5.386	25.570
40.00	1.003	2.309	3.312	92.369	6.559	40.118
45.00	1.306	2.842	4.148	127.88	7.641	58.756
50.00	1.633	3.376	5.009	168.82	8.733	81.637
55.00	1.980	3.909	5.889	215.01	9.711	108.88
60.00	2.342	4.429	6.771	265.72	10.567	140.53
65.00	2.717	4.933	7.650	320.66	11.402	176.58
70.00	3.100	5.422	8.523	379.57	12.143	217.02
75.00	3.490	5.893	9.383	441.94	12.801	261.79
80.00	3.885	6.345	10.230	507.61	13.468	310.83
85.00	4.283	6.783	11.066	576.56	14.099	364.07
90.00	4.683	7.205	11.888	648.48	14.666	421.47
95.00	5.083	7.613	12.696	723.21	15.222	482.93
100.00	5.484	8.006	13.490	800.61	15.724	548.40
105.00	5.884	8.384	14.268	880.34	16.168	617.81
110.00	6.282	8.749	15.031	962.38	16.654	691.06
115.00	6.679	9.103	15.782	1046.9	17.142	768.10
120.00	7.074	9.448	16.522	1133.7	17.580	848.86
125.00	7.466	9.780	17.247	1222.6	17.946	933.29
130.00	7.856	10.101	17.958	1313.2	18.303	1021.3
135.00	8.243	10.411	18.655	1405.5	18.631	1112.8
140.00	8.627	10.711	19.338	1499.5	18.947	1207.8
145.00	9.008	11.000	20.008	1595.0	19.259	1306.2
150.00	9.386	11.280	20.666	1692.0	19.562	1407.9
155.00	9.760	11.552	21.313	1790.6	19.861	1512.8
160.00	10.131	11.817	21.948	1890.7	20.155	1621.0
165.00	10.499	12.074	22.572	1992.1	20.442	1732.3
170.00	10.863	12.324	23.187	2095.1	20.725	1846.7
175.00	11.224	12.568	23.792	2199.4	21.002	1964.2
180.00	11.581	12.806	24.387	2305.1	21.274	2084.6
185.00	11.935	13.038	24.974	2412.1	21.538	2208.0
190.00	12.286	13.265	25.551	2520.4	21.792	2334.3
195.00	12.633	13.487	26.121	2630.0	22.033	2463.5
200.00	12.978	13.704	26.681	2740.7	22.260	2595.5
205.00	13.319	13.915	27.234	2852.6	22.472	2730.3
210.00	13.656	14.121	27.778	2965.4	22.667	2867.8
215.00	13.991	14.322	28.313	3079.2	22.850	3008.1
220.00	14.323	14.518	28.840	3193.9	23.022	3151.0
225.00	14.651	14.709	29.360	3309.4	23.187	3296.5
230.00	14.976	14.895	29.871	3425.8	23.347	3444.5
235.00	15.299	15.076	30.375	3542.9	23.507	3595.2
240.00	15.618	15.254	30.871	3660.8	23.666	3748.3
245.00	15.934	15.427	31.361	3779.6	23.825	3903.9
250.00	16.248	15.596	31.844	3899.1	23.985	4061.9
255.00	16.558	15.762	32.320	4019.4	24.143	4222.3
260.00	16.866	15.925	32.791	4140.5	24.300	4385.1
265.00	17.171	16.085	33.255	4262.4	24.452	4550.2
270.00	17.473	16.241	33.714	4385.0	24.599	4717.6
273.15	17.662	16.338	33.999	4462.7	24.689	4824.3
275.00	17.772	16.394	34.166	4508.4	24.740	4887.3
280.00	18.069	16.544	34.613	4632.4	24.875	5059.3
285.00	18.363	16.692	35.055	4757.1	25.002	5233.4
290.00	18.654	16.836	35.490	4882.4	25.123	5409.4
295.00	18.944	16.977	35.921	5008.3	25.238	5588.3
298.15	19.124	17.065	36.189	5088.0	25.307	5701.9
300.00	19.230	17.116	36.346	5134.8	25.346	5769.0

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

TABLE 9-98

THERMODYNAMIC FUNCTIONS FOR AMMONIUM OXIDE ((NH_4)$_2$O)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=52.07656 GRAMS   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	$\dfrac{CAL}{DEG\text{-}MOLE}$	$\dfrac{CAL}{DEG\text{-}MOLE}$	$\dfrac{CAL}{DEG\text{-}MOLE}$	$\dfrac{CAL}{MOLE}$	$\dfrac{CAL}{DEG\text{-}MOLE}$	$\dfrac{CAL}{MOLE}$
			SOLID PHASE			
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.004	0.011	0.014	0.053	0.042	0.018
10.00	0.028	0.085	0.113	0.849	0.339	0.283
15.00	0.095	0.281	0.376	4.211	1.082	1.425
20.00	0.218	0.611	0.829	12.214	2.150	4.362
25.00	0.399	1.037	1.435	25.920	3.348	9.968
30.00	0.630	1.529	2.159	45.865	4.649	18.911
35.00	0.906	2.073	2.979	72.552	6.022	31.721
40.00	1.220	2.643	3.863	105.72	7.197*	48.811
45.00	1.564	3.206	4.771	144.29	8.236*	70.390
50.00	1.931	3.762	5.693	188.08	9.262*	96.557
50.00	1.931	4.675	6.606	233.73	9.262*	96.557
55.00	2.398	5.132	7.530	282.25	10.133*	131.91
60.00	2.864	5.583	8.447	334.98	10.957	171.86
65.00	3.329	6.029	9.358	391.89	11.799	216.38
70.00	3.792	6.467	10.259	452.71	12.514	265.42
75.00	4.253	6.893	11.145	516.45	13.180	318.94
80.00	4.711	7.307	12.018	584.57	13.870	376.85
85.00	5.166	7.714	12.879	655.65	14.562	439.10
90.00	5.618	8.113	13.731	730.19	15.250	505.63
95.00	6.067	8.507	14.574	808.13	15.925	576.40
100.00	6.514	8.894	15.408	889.42	16.590	651.36
105.00	6.957	9.276	16.233	974.00	17.240	730.46
110.00	7.397	9.653	17.050	1061.8	17.893	813.67
115.00	7.834	10.025	17.859	1152.4	18.508	900.95
120.00	8.269	10.391	18.659	1246.9	19.103	992.25
125.00	8.700	10.751	19.451	1343.9	19.693	1087.5
130.00	9.129	11.106	20.235	1443.8	20.266	1186.7
135.00	9.555	11.456	21.010	1546.5	20.832	1289.9
140.00	9.977	11.801	21.778	1652.1	21.392	1396.8
145.00	10.397	12.141	22.538	1760.4	21.945	1507.6
150.00	10.815	12.477	23.292	1871.5	22.492	1622.2
155.00	11.229	12.809	24.038	1985.3	23.032	1740.5
160.00	11.641	13.137	24.778	2101.8	23.565	1862.6
165.00	12.050	13.461	25.511	2221.0	24.091	1988.3
170.00	12.457	13.781	26.238	2342.7	24.613	2117.7
175.00	12.861	14.098	26.959	2467.1	25.133	2250.7
180.00	13.263	14.412	27.674	2594.1	25.655	2387.3
185.00	13.662	14.723	28.384	2723.7	26.185	2527.4
190.00	14.058	15.031	29.090	2855.0	26.725	2671.1
194.31	14.398	15.296	29.694	2972.2	27.204	2797.8
			LIQUID PHASE			
194.31	14.398	27.400	41.799	5324.2	46.923	2797.8
195.00	14.495	27.470	41.965	5356.6	46.999	2826.7
200.00	15.197	27.965	43.162	5592.9	47.547	3039.5
205.00	15.894	28.449	44.343	5832.0	48.089	3258.3
210.00	16.585	28.923	45.508	6073.8	48.625	3482.9
215.00	17.271	29.387	46.658	6318.3	49.153	3713.3
220.00	17.952	29.842	47.794	6565.3	49.674	3949.5
225.00	18.628	30.289	48.917	6815.0	50.186	4191.2
230.00	19.298	30.727	50.025	7067.2	50.689	4438.6
235.00	19.964	31.157	51.120	7321.0	51.182	4691.5
240.00	20.624	31.579	52.203	7579.0	51.666	4949.8
245.00	21.279	31.994	53.273	7838.5	52.138	5213.5
250.00	21.930	32.401	54.331	8100.3	52.600	5482.5
255.00	22.576	32.802	55.377	8364.5	53.049	5756.8
260.00	23.216	33.195	56.412	8630.8	53.486	6036.2
265.00	23.852	33.582	57.435	8899.3	53.910	6320.9
270.00	24.484	33.963	58.446	9169.9	54.319	6610.6
273.15	24.879	34.199	59.078	9341.4	54.570	6795.7
275.00	25.110	34.336	59.446	9442.5	54.715	6905.2
280.00	25.732	34.704	60.436	9717.0	55.096	7205.0
285.00	26.350	35.065	61.414	9993.4	55.461	7509.6
290.00	26.963	35.419	62.382	10272.	55.811	7819.1
295.00	27.571	35.768	63.339	10551.	56.143	8133.4
298.15	27.952	35.984	63.936	10729.	56.344	8333.8
300.00	28.175	36.110	64.285	10833.	56.459	8452.5

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

* HYPOTHETICAL HEAT CAPACITIES IN THE RANGE OF THE TRANSITION

TABLE R-99

THERMODYNAMIC FUNCTIONS FOR AMMONIUM HYDROXIDE (N H$_4$O H)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=87.12251 GRAMS   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

T						
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.004	0.005	0.019	0.015	0.006
10.00	0.010	0.030	0.041	0.304	0.122	0.101
15.00	0.034	0.103	0.137	1.546	0.413	0.514
20.00	0.081	0.241	0.322	4.814	0.924	1.622
25.00	0.155	0.438	0.593	10.939	1.532	3.877
30.00	0.255	0.673	0.928	20.183	2.174	7.655
35.00	0.378	0.936	1.314	32.759	2.862	13.241
40.00	0.522	1.220	1.741	48.787	3.540	20.866
45.00	0.682	1.513	2.196	68.101	4.185	30.699
50.00	0.857	1.813	2.670	90.662	4.841	42.856
55.00	1.044	2.118	3.162	116.48	5.482	57.431
60.00	1.242	2.424	3.666	145.46	6.111	74.497
65.00	1.448	2.732	4.180	177.59	6.735	94.108
70.00	1.662	3.040	4.701	212.78	7.337	116.31
75.00	1.882	3.346	5.227	250.93	7.921	141.13
80.00	2.107	3.649	5.757	291.94	8.479	168.59
85.00	2.338	3.950	6.287	335.72	9.033	198.70
90.00	2.572	4.247	6.819	382.26	9.581	231.46
95.00	2.809	4.542	7.351	431.50	10.115	266.89
100.00	3.050	4.834	7.884	483.39	10.637	304.98
105.00	3.293	5.122	8.415	537.86	11.152	345.72
110.00	3.538	5.408	8.946	594.91	11.668	389.13
115.00	3.784	5.691	9.475	654.50	12.163	435.18
120.00	4.032	5.971	10.003	716.53	12.652	483.88
125.00	4.282	6.248	10.530	780.98	13.127	535.21
130.00	4.532	6.521	11.054	847.79	13.596	589.17
135.00	4.783	6.792	11.575	916.93	14.060	645.74
140.00	5.035	7.060	12.095	988.38	14.520	704.92
145.00	5.288	7.325	12.613	1062.1	14.980	766.69
150.00	5.540	7.588	13.128	1138.2	15.439	831.04
155.00	5.793	7.849	13.642	1216.5	15.897	897.97
160.00	6.047	8.107	14.154	1297.2	16.354	967.46
165.00	6.300	8.364	14.664	1380.1	16.808	1039.5
170.00	6.553	8.619	15.173	1465.2	17.260	1114.1
175.00	6.807	8.872	15.679	1552.7	17.708	1191.2
180.00	7.060	9.124	16.184	1642.3	18.152	1270.9
185.00	7.314	9.374	16.688	1734.2	19.592	1353.1
190.00	7.567	9.622	17.189	1828.2	19.028	1437.8
194.14	7.777	9.827	17.603	1907.7	19.386	1509.8

LIQUID PHASE

T						
194.14	7.777	17.903	25.680	3475.7	28.081	1509.8
195.00	7.856	17.948	25.804	3499.9	28.155	1531.9
200.00	8.314	18.209	26.522	3641.7	28.591	1662.7
205.00	8.766	18.467	27.234	3785.8	29.033	1797.1
210.00	9.214	18.724	27.939	3932.1	29.480	1935.0
215.00	9.658	18.980	28.638	4080.6	29.930	2076.5
220.00	10.097	19.234	29.331	4231.4	30.383	2221.4
225.00	10.532	19.486	30.019	4384.4	30.838	2369.8
230.00	10.963	19.738	30.701	4539.8	31.293	2521.6
235.00	11.391	19.989	31.379	4697.4	31.747	2676.8
240.00	11.814	20.238	32.052	4857.2	32.200	2835.4
245.00	12.234	20.487	32.721	5019.4	32.650	2997.3
250.00	12.650	20.735	33.385	5183.7	33.096	3162.6
255.00	13.063	20.982	34.045	5350.3	33.537	3331.1
260.00	13.473	21.227	34.700	5519.1	33.973	3503.0
265.00	13.880	21.472	35.352	5690.0	34.401	3678.1
270.00	14.283	21.715	35.999	5863.1	34.822	3856.5
273.15	14.536	21.868	36.404	5973.2	35.082	3970.5
275.00	14.684	21.957	36.641	6038.2	35.233	4038.1
280.00	15.082	22.198	37.280	6215.4	35.634	4222.9
285.00	15.477	22.437	37.914	6394.6	36.025	4410.9
290.00	15.869	22.675	38.544	6575.6	36.402	4602.0
295.00	16.259	22.910	39.169	6758.6	36.767	4796.3
298.15	16.503	23.058	39.561	6874.7	36.989	4920.3
300.00	16.646	23.144	39.790	6943.3	37.117	4993.7

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

TABLE B-100

THERMODYNAMIC FUNCTIONS FOR AMMONIUM FLUORIDE (N H$_4$ F)
SOLID PHASE

GRAM MOLECULAR WT.=37.03698 GRAMS   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	0.001	0.003	0.004	0.015	0.012	0.005
10.00	0.008	0.022	0.030	0.224	0.089	0.077
15.00	0.026	0.078	0.104	1.176	0.322	0.385
20.00	0.062	0.184	0.245	3.678	0.692	1.232
25.00	0.117	0.327	0.445	8.181	1.113	2.937
30.00	0.192	0.494	0.686	14.819	1.539	5.748
35.00	0.281	0.673	0.954	23.541	1.945	9.837
40.00	0.383	0.855	1.238	34.219	2.323	15.312
45.00	0.494	1.040	1.534	46.782	2.705	22.238
50.00	0.613	1.225	1.838	61.251	3.082	30.665
55.00	0.739	1.412	2.151	77.654	3.487	40.634
60.00	0.870	1.601	2.471	96.080	3.871	52.186
65.00	1.005	1.789	2.795	116.31	4.227	65.349
70.00	1.145	1.977	3.122	138.41	4.614	80.140
75.00	1.288	2.166	3.453	162.43	4.996	96.577
80.00	1.433	2.355	3.788	188.37	5.379	114.68
85.00	1.582	2.544	4.126	216.21	5.756	134.46
90.00	1.733	2.732	4.465	245.90	6.115	155.94
95.00	1.885	2.919	4.805	277.33	6.458	179.11
100.00	2.040	3.105	5.144	310.46	6.793	203.99
105.00	2.196	3.288	5.484	345.27	7.131	230.56
110.00	2.353	3.471	5.824	381.76	7.464	258.83
115.00	2.511	3.651	6.162	419.88	7.784	288.79
120.00	2.670	3.830	6.500	459.60	8.104	320.45
125.00	2.830	4.007	6.837	500.89	8.409	353.79
130.00	2.991	4.182	7.173	543.68	8.708	388.82
135.00	3.152	4.355	7.507	587.96	9.001	425.52
140.00	3.314	4.526	7.840	633.68	9.286	463.89
145.00	3.475	4.695	8.171	680.81	9.565	503.92
150.00	3.637	4.862	8.499	729.32	9.837	545.59
155.00	3.799	5.027	8.826	779.17	10.102	588.91
160.00	3.962	5.190	9.151	830.33	10.359	633.85
165.00	4.124	5.350	9.474	882.75	10.608	680.42
170.00	4.286	5.508	9.794	936.40	10.851	728.59
175.00	4.448	5.664	10.112	991.24	11.087	778.35
180.00	4.609	5.818	10.428	1047.3	11.317	829.70
185.00	4.771	5.970	10.741	1104.4	11.542	882.62
190.00	4.932	6.119	11.051	1162.7	11.761	937.11
195.00	5.093	6.267	11.360	1222.0	11.975	993.13
200.00	5.253	6.412	11.666	1282.4	12.184	1050.7
205.00	5.414	6.555	11.969	1343.8	12.389	1109.8
210.00	5.573	6.697	12.270	1406.3	12.589	1170.4
215.00	5.732	6.836	12.568	1469.7	12.786	1232.5
220.00	5.891	6.973	12.865	1534.1	12.979	1296.1
225.00	6.049	7.109	13.158	1599.5	13.169	1361.1
230.00	6.207	7.243	13.450	1665.8	13.356	1427.6
235.00	6.364	7.375	13.739	1733.1	13.541	1495.6
240.00	6.521	7.505	14.026	1801.2	13.722	1565.0
245.00	6.677	7.634	14.311	1870.3	13.900	1635.9
250.00	6.833	7.761	14.593	1940.2	14.073	1708.1
255.00	6.987	7.886	14.874	2011.0	14.243	1781.8
260.00	7.142	8.010	15.152	2082.6	14.409	1856.9
265.00	7.296	8.132	15.428	2155.1	14.572	1933.3
270.00	7.449	8.253	15.702	2228.4	14.732	2011.1
273.15	7.545	8.328	15.873	2274.9	14.832	2060.9
275.00	7.601	8.372	15.974	2302.4	14.890	2090.3
280.00	7.753	8.490	16.243	2377.3	15.047	2170.9
285.00	7.904	8.607	16.511	2452.9	15.202	2252.8
290.00	8.055	8.722	16.777	2529.3	15.356	2336.0
295.00	8.205	8.835	17.041	2606.4	15.508	2420.5
298.15	8.299	8.906	17.206	2655.4	15.604	2474.5
300.00	8.355	8.948	17.302	2684.4	15.660	2506.4

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

TABLE B-101

THERMODYNAMIC FUNCTIONS FOR AMMONIUM FLUORIDE MONOHYDRATE (N H$_4$F ·H$_2$O)
SOLID PHASE

GRAM MOLECULAR WT.=55.05232 GRAMS   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	0.001	0.003	0.004	0.014	0.012	0.004
10.00	0.009	0.034	0.043	0.338	0.159	0.094
15.00	0.040	0.138	0.178	2.074	0.578	0.600
20.00	0.103	0.324	0.427	6.472	1.205	2.067
25.00	0.201	0.569	0.770	14.224	1.898	5.027
30.00	0.329	0.848	1.177	25.432	2.581	9.874
35.00	0.482	1.142	1.624	39.975	3.230	16.863
40.00	0.654	1.442	2.095	57.665	3.840	26.153
45.00	0.841	1.741	2.582	78.339	4.429	37.841
50.00	1.040	2.039	3.079	101.95	5.014	51.989
55.00	1.248	2.336	3.584	128.48	5.598	68.643
60.00	1.464	2.632	4.096	157.92	6.174	87.841
65.00	1.686	2.926	4.613	190.20	6.738	109.61
70.00	1.914	3.219	5.132	225.30	7.297	133.97
75.00	2.146	3.509	5.655	263.17	7.852	160.94
80.00	2.382	3.798	6.179	303.84	8.419	190.52
85.00	2.620	4.087	6.707	347.35	8.983	222.74
90.00	2.862	4.373	7.235	393.60	9.508	257.59
95.00	3.106	4.657	7.763	442.38	10.002	295.09
100.00	3.352	4.936	8.289	493.63	10.502	335.22
105.00	3.600	5.213	8.813	547.40	11.002	377.97
110.00	3.849	5.487	9.336	603.62	11.482	423.35
115.00	4.099	5.758	9.857	662.20	11.947	471.33
120.00	4.349	6.026	10.375	723.08	12.406	521.91
125.00	4.601	6.290	10.891	786.26	12.864	575.08
130.00	4.852	6.552	11.404	851.70	13.311	630.81
135.00	5.105	6.810	11.915	919.36	13.750	689.11
140.00	5.357	7.066	12.422	989.18	14.178	749.95
145.00	5.609	7.318	12.927	1061.1	14.597	813.33
150.00	5.861	7.568	13.429	1135.1	15.007	879.22
155.00	6.114	7.814	13.928	1211.2	15.410	947.62
160.00	6.366	8.058	14.423	1289.2	15.810	1018.5
165.00	6.617	8.299	14.916	1369.3	16.208	1091.8
170.00	6.869	8.537	15.406	1451.3	16.608	1167.6
175.00	7.119	8.773	15.893	1535.4	17.010	1245.9
180.00	7.370	9.008	16.378	1621.4	17.413	1326.6
185.00	7.620	9.240	16.860	1709.5	17.815	1409.7
190.00	7.869	9.471	17.341	1799.6	18.212	1495.2
195.00	8.118	9.700	17.819	1891.6	18.603	1583.1
200.00	8.367	9.928	18.295	1985.6	18.983	1673.4
205.00	8.615	10.153	18.768	2081.4	19.353	1766.0
210.00	8.862	10.377	19.239	2179.1	19.712	1861.0
215.00	9.109	10.598	19.707	2278.5	20.063	1958.4
220.00	9.355	10.817	20.172	2379.7	20.408	2058.1
225.00	9.600	11.034	20.634	2482.6	20.749	2160.1
230.00	9.845	11.249	21.094	2587.2	21.087	2264.4
235.00	10.090	11.461	21.551	2693.4	21.422	2371.0
240.00	10.333	11.672	22.005	2801.4	21.753	2479.9
245.00	10.576	11.881	22.457	2911.0	22.079	2591.1
246.00	10.624	11.923	22.547	2933.1	22.143	2613.6
246.00	10.624	17.481	28.105	4300.4	33.302	2613.6
250.00	10.908	17.737	28.644	4434.2	33.578	2727.0
255.00	11.262	18.051	29.313	4602.9	33.939	2871.9
260.00	11.616	18.360	29.976	4773.6	34.317	3020.1
265.00	11.968	18.665	30.633	4946.1	34.711	3171.6
270.00	12.320	18.966	31.286	5120.7	35.124	3326.4
273.15	12.541	19.154	31.695	5231.8	35.393	3425.6
275.00	12.671	19.263	31.934	5297.4	35.555	3484.5
280.00	13.020	19.558	32.579	5476.3	36.006	3645.7
285.00	13.369	19.851	33.220	5657.5	36.477	3810.2
290.00	13.717	20.142	33.859	5841.1	36.968	3977.9
295.00	14.064	20.431	34.495	6027.2	37.481	4148.8
298.15	14.282	20.613	34.895	6145.8	37.815	4258.1
300.00	14.410	20.720	35.129	6215.9	38.016	4322.9

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

TABLE B-102

THERMODYNAMIC FUNCTIONS FOR NITRIC ACID (H N O$_3$)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=63.01287 GRAMS   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

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	$-(G^0_T-H^0_0)$
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.002	0.006	0.008	0.032	0.025	0.011
10.00	0.017	0.051	0.068	0.511	0.207	0.169
15.00	0.058	0.174	0.232	2.609	0.677	0.866
20.00	0.134	0.373	0.506	7.453	1.264	2.674
25.00	0.242	0.616	0.859	15.412	1.944	6.057
30.00	0.379	0.903	1.283	27.095	2.746	11.381
35.00	0.543	1.230	1.773	43.059	3.646	18.993
40.00	0.730	1.585	2.315	63.389	4.460	29.197
45.00	0.937	1.945	2.882	87.525	5.191	42.182
50.00	1.161	2.304	3.465	115.21	5.866	58.046
55.00	1.397	2.656	4.053	146.05	6.464	76.840
60.00	1.643	2.996	4.639	179.77	7.015	98.570
65.00	1.896	3.325	5.221	216.13	7.523	123.22
70.00	2.154	3.642	5.795	254.91	7.977	150.77
75.00	2.415	3.945	6.360	295.85	8.398	181.16
80.00	2.679	4.236	6.915	338.88	8.814	214.35
85.00	2.945	4.517	7.461	383.93	9.192	250.30
90.00	3.211	4.785	7.996	430.69	9.503	288.95
95.00	3.476	5.041	8.517	478.90	9.782	330.23
100.00	3.741	5.285	9.026	528.53	10.067	374.10
105.00	4.005	5.519	9.524	579.54	10.332	420.48
110.00	4.267	5.744	10.010	631.79	10.566	469.32
115.00	4.527	5.958	10.485	685.20	10.796	520.56
120.00	4.785	6.164	10.949	739.74	11.017	574.15
125.00	5.040	6.363	11.403	795.39	11.246	630.04
130.00	5.294	6.555	11.849	852.19	11.471	688.17
135.00	5.545	6.742	12.286	910.11	11.697	748.51
140.00	5.793	6.923	12.716	969.16	11.923	811.02
145.00	6.039	7.099	13.138	1029.3	12.147	875.65
150.00	6.283	7.271	13.553	1090.6	12.371	942.38
155.00	6.524	7.439	13.963	1153.0	12.594	1011.2
160.00	6.763	7.604	14.366	1216.6	12.816	1082.0
165.00	6.999	7.765	14.764	1281.2	13.039	1154.8
170.00	7.233	7.923	15.156	1347.0	13.263	1229.6
175.00	7.465	8.079	15.544	1413.8	13.490	1306.4
180.00	7.695	8.233	15.927	1481.9	13.719	1385.1
185.00	7.922	8.384	16.306	1551.0	13.948	1465.7
190.00	8.148	8.533	16.681	1621.3	14.177	1548.1
195.00	8.372	8.681	17.053	1692.8	14.405	1632.5
200.00	8.593	8.827	17.420	1765.4	14.636	1718.6
205.00	8.813	8.972	17.785	1839.2	14.879	1806.7
210.00	9.031	9.115	18.146	1914.2	15.151	1896.5
215.00	9.247	9.259	18.506	1990.8	15.477	1988.1
220.00	9.462	9.404	18.866	2069.0	15.803	2081.5
225.00	9.674	9.550	19.224	2148.8	16.129	2176.6
230.00	9.885	9.697	19.582	2230.3	16.455	2273.6
231.50	9.949	9.741	19.690	2255.1	16.553	2303.1

LIQUID PHASE

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	$-(G^0_T-H^0_0)$
231.50	9.949	20.553	30.502	4758.1	26.752	2303.1
235.00	10.257	20.646	30.903	4851.7	26.733	2410.5
240.00	10.694	20.772	31.465	4985.3	26.705	2566.6
245.00	11.123	20.893	32.016	5118.7	26.674	2725.2
250.00	11.546	21.008	32.554	5252.0	26.641	2886.5
255.00	11.964	21.118	33.082	5385.2	26.605	3050.7
260.00	12.375	21.223	33.598	5518.1	26.568	3217.4
265.00	12.780	21.324	34.104	5650.8	26.528	3386.8
270.00	13.179	21.420	34.599	5783.4	26.485	3558.3
273.15	13.428	21.478	34.906	5866.8	26.458	3667.8
275.00	13.573	21.512	35.085	5915.7	26.441	3732.7
280.00	13.962	21.599	35.561	6047.8	26.394	3909.3
285.00	14.345	21.683	36.028	6179.6	26.345	4088.4
290.00	14.723	21.763	36.486	6311.2	26.293	4269.7
295.00	15.096	21.839	36.935	6442.5	26.239	4453.3
298.15	15.328	21.885	37.213	6525.1	26.204	4570.0
300.00	15.463	21.912	37.375	6573.6	26.183	4638.9

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

TABLE B-103

THERMODYNAMIC FUNCTIONS FOR NITRIC ACID MONOHYDRATE (H N O$_3$·H$_2$O) SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=81.02821 GRAMS   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			
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.002	0.006	0.008	0.030	0.024	0.010
10.00	0.016	0.047	0.063	0.473	0.189	0.158
15.00	0.053	0.157	0.210	2.351	0.605	0.794
20.00	0.122	0.344	0.465	6.870	1.229	2.438
25.00	0.224	0.594	0.819	14.854	1.978	5.611
30.00	0.359	0.893	1.251	26.782	2.814	10.756
35.00	0.521	1.235	1.756	43.222	3.775	18.245
40.00	0.711	1.611	2.322	64.455	4.693	28.420
45.00	0.923	1.999	2.922	89.951	5.497	41.519
50.00	1.153	2.389	3.542	119.45	6.309	57.670
55.00	1.400	2.783	4.182	153.04	7.121	76.975
60.00	1.659	3.176	4.834	190.54	7.865	99.513
65.00	1.928	3.563	5.491	231.59	8.543	125.32
70.00	2.206	3.941	6.147	275.85	9.151	154.42
75.00	2.499	4.308	6.798	323.08	9.750	186.78
80.00	2.780	4.668	7.448	373.41	10.378	222.40
85.00	3.074	5.021	8.094	426.77	10.956	261.26
90.00	3.370	5.365	8.735	482.81	11.432	303.33
95.00	3.669	5.693	9.363	540.86	11.787	348.58
100.00	3.969	6.009	9.978	600.90	12.256	396.94
105.00	4.270	6.319	10.589	663.49	12.765	448.36
110.00	4.571	6.621	11.192	728.32	13.151	502.82
115.00	4.872	6.913	11.784	794.94	13.499	560.26
120.00	5.172	7.194	12.367	863.34	13.863	620.64
125.00	5.471	7.468	12.940	933.54	14.216	683.91
130.00	5.769	7.734	13.504	1005.5	14.560	750.02
135.00	6.066	7.994	14.060	1079.1	14.899	818.94
140.00	6.361	8.246	14.608	1154.5	15.229	890.61
145.00	6.655	8.492	15.148	1231.4	15.551	965.00
150.00	6.947	8.733	15.680	1310.0	15.866	1042.1
155.00	7.237	8.968	16.205	1390.1	16.173	1121.8
160.00	7.526	9.198	16.724	1471.7	16.474	1204.1
165.00	7.812	9.423	17.235	1554.8	16.767	1289.0
170.00	8.097	9.643	17.740	1639.3	17.055	1376.5
175.00	8.379	9.859	18.238	1725.3	17.338	1466.4
180.00	8.660	10.071	18.731	1812.7	17.621	1558.8
185.00	8.939	10.279	19.217	1901.5	17.905	1653.7
190.00	9.216	10.483	19.699	1991.8	18.191	1751.0
195.00	9.491	10.684	20.175	2083.5	18.479	1850.7
200.00	9.764	10.883	20.647	2176.6	18.765	1952.7
205.00	10.035	11.079	21.113	2271.1	19.044	2057.1
210.00	10.304	11.271	21.575	2367.0	19.309	2163.9
215.00	10.572	11.461	22.033	2464.2	19.556	2272.9
220.00	10.837	11.648	22.485	2562.5	19.780	2384.2
225.00	11.101	11.831	22.932	2661.9	19.981	2497.7
230.00	11.363	12.010	23.373	2762.3	20.157	2613.5
235.00	11.623	12.185	23.808	2863.4	20.308	2731.4
235.47	11.648	12.201	23.849	2873.0	20.320	2742.6
			LIQUID PHASE			
235.47	11.648	29.970	41.618	7057.0	42.995	2742.6
240.00	12.221	30.216	42.437	7251.8	43.009	2933.1
245.00	12.847	30.477	43.324	7466.9	43.042	3147.5
250.00	13.465	30.729	44.194	7682.2	43.092	3366.3
255.00	14.076	30.972	45.048	7897.9	43.154	3589.4
260.00	14.680	31.207	45.887	8113.8	43.225	3816.8
265.00	15.277	31.434	46.711	8330.1	43.301	4048.3
270.00	15.866	31.655	47.521	8546.8	43.379	4283.9
273.15	16.234	31.790	48.024	8683.5	43.427	4434.4
275.00	16.449	31.869	48.318	8763.9	43.454	4523.5
280.00	17.025	32.076	49.101	8981.0	43.524	4767.0
285.00	17.595	32.278	49.872	9199.1	43.585	5014.5
290.00	18.158	32.473	50.631	9417.2	43.632	5265.7
295.00	18.714	32.662	51.377	9635.4	43.663	5520.7
298.15	19.062	32.779	51.841	9773.0	43.672	5683.3
300.00	19.265	32.846	52.111	9853.8	43.673	5779.5

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

TABLE B-104

THERMODYNAMIC FUNCTIONS FOR NITRIC ACID TRIHYDRATE (H N O$_3$ .3H$_2$O)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.=117.05889 GRAMS   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

T						
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.003	0.009	0.012	0.046	0.037	0.015
10.00	0.024	0.073	0.098	0.732	0.293	0.244
15.00	0.082	0.243	0.326	3.652	0.951	1.230
20.00	0.190	0.546	0.737	10.926	2.014	3.808
25.00	0.356	0.966	1.321	24.142	3.286	8.888
30.00	0.576	1.472	2.048	44.166	4.770	17.274
35.00	0.844	2.057	2.901	72.000	6.361	29.535
40.00	1.162	2.689	3.851	107.57	7.856	46.470
45.00	1.516	3.336	4.852	150.12	9.125	68.220
50.00	1.900	3.982	5.882	199.08	10.471	95.020
55.00	2.311	4.632	6.943	254.78	11.797	127.08
60.00	2.742	5.279	8.021	316.74	12.951	164.52
65.00	3.190	5.909	9.099	384.10	13.987	207.34
70.00	3.651	6.522	10.172	456.54	14.987	255.55
75.00	4.120	7.121	11.241	534.08	16.044	309.00
80.00	4.599	7.711	12.310	616.91	17.059	367.89
85.00	5.083	8.288	13.371	704.46	17.953	432.08
90.00	5.573	8.849	14.422	796.42	18.823	501.56
95.00	6.066	9.395	15.461	892.52	19.601	576.28
100.00	6.562	9.924	16.486	992.10	20.360	656.20
105.00	7.059	10.439	17.498	1096.1	21.116	741.19
110.00	7.556	10.941	18.497	1203.5	21.847	831.17
115.00	8.054	11.430	19.484	1314.5	22.539	926.16
120.00	8.549	11.906	20.456	1428.8	23.171	1025.9
125.00	9.045	12.371	21.416	1546.4	23.865	1130.6
130.00	9.539	12.826	22.365	1667.4	24.523	1240.0
135.00	10.032	13.271	23.303	1791.6	25.179	1354.3
140.00	10.521	13.708	24.230	1919.2	25.833	1473.0
145.00	11.011	14.137	25.148	2049.9	26.472	1596.6
150.00	11.597	14.559	26.156	2183.9	27.106	1739.5
155.00	11.981	14.974	26.955	2321.0	27.733	1857.0
160.00	12.464	15.382	27.846	2461.2	28.354	1994.2
165.00	12.943	15.785	28.728	2604.5	28.972	2135.6
170.00	13.420	16.182	29.602	2750.9	29.587	2281.4
175.00	13.894	16.574	30.468	2900.4	30.201	2431.5
180.00	14.367	16.960	31.328	3052.9	30.811	2586.1
185.00	14.837	17.343	32.180	3208.5	31.418	2744.8
190.00	15.304	17.721	33.026	3367.1	32.016	2907.8
195.00	15.770	18.095	33.865	3528.6	32.601	3075.1
200.00	16.233	18.465	34.698	3693.0	33.168	3246.6
205.00	16.692	18.831	35.523	3860.3	33.715	3421.9
210.00	17.151	19.191	36.342	4030.2	34.246	3601.6
215.00	17.578	19.548	37.126	4202.8	34.805	3779.3
220.00	18.007	19.901	37.908	4378.2	35.431	3961.6
225.00	18.428	20.255	38.683	4557.4	36.125	4146.3
230.00	18.850	20.607	39.457	4739.7	36.887	4335.4
235.00	19.269	20.963	40.232	4926.4	37.716	4528.1
240.00	19.685	21.322	41.007	5117.2	38.613	4724.5
245.00	20.109	21.683	41.792	5312.4	39.577	4926.6
250.00	20.521	22.053	42.574	5513.3	40.610	5130.2
254.62	21.144	22.398	43.543	5703.1	41.624	5383.8

LIQUID PHASE

T						
254.62	21.144	49.709	70.854	12657.	74.460	5383.8
255.00	21.220	49.745	70.965	12685.	74.502	5411.1
260.00	22.190	50.227	72.417	13059.	75.036	5769.4
265.00	23.153	50.698	73.851	13435.	75.527	6135.5
270.00	24.104	51.163	75.267	13814.	75.974	6508.1
273.15	24.698	51.452	76.150	14054.	76.234	6746.4
275.00	25.047	51.618	76.665	14195.	76.379	6887.9
280.00	25.981	52.064	78.045	14578.	76.740	7274.6
285.00	26.908	52.498	79.406	14962.	77.059	7668.7
290.00	27.824	52.924	80.748	15348.	77.333	8068.9
295.00	28.730	53.342	82.072	15736.	77.564	8475.2
298.15	29.300	53.597	82.897	15980.	77.687	8735.7
300.00	29.631	53.747	83.378	16124.	77.752	8889.4

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

TABLE B-105

THERMODYNAMIC FUNCTIONS FOR MERCURIC OXIDE (RED) (HG O)
SOLID PHASE

GRAM MOLECULAR WT.=216.5894 GRAMS   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	$\frac{CAL}{DEG\ MOLE}$	$\frac{CAL}{DEG\ MOLE}$	$\frac{CAL}{DEG\ MOLE}$	$\frac{CAL}{MOLE}$	$\frac{CAL}{DEG\ MOLE}$	$\frac{CAL}{MOLE}$
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.002	0.007	0.009	0.036	0.028	0.012
10.00	0.019	0.057	0.076	0.566	0.225	0.189
15.00	0.063	0.189	0.252	2.832	0.747	0.952
20.00	0.148	0.428	0.576	8.555	1.551	2.963
25.00	0.275	0.723	0.998	18.071	2.224	6.875
30.00	0.433	1.023	1.456	30.693	2.828	12.999
35.00	0.614	1.323	1.937	46.319	3.408	21.476
40.00	0.810	1.615	2.425	64.601	3.890	32.380
45.00	1.016	1.891	2.907	85.094	4.295	45.713
50.00	1.229	2.149	3.378	107.45	4.642	61.429
55.00	1.445	2.390	3.835	131.46	4.955	79.466
60.00	1.663	2.615	4.278	156.93	5.224	99.755
65.00	1.880	2.825	4.706	183.66	5.465	122.22
70.00	2.097	3.022	5.119	211.54	5.679	146.79
75.00	2.312	3.205	5.517	240.41	5.873	173.39
80.00	2.524	3.379	5.904	270.35	6.108	201.94
85.00	2.734	3.546	6.281	301.44	6.321	232.41
90.00	2.941	3.706	6.647	333.53	6.519	264.73
95.00	3.146	3.859	7.005	366.63	6.716	298.86
100.00	3.348	4.006	7.354	400.64	6.880	334.77
105.00	3.547	4.146	7.693	435.38	7.010	372.39
110.00	3.743	4.279	8.022	470.71	7.119	411.68
115.00	3.936	4.405	8.341	506.57	7.229	452.59
120.00	4.126	4.525	8.651	543.03	7.358	495.07
125.00	4.313	4.641	8.954	580.14	7.487	539.09
130.00	4.497	4.753	9.250	617.90	7.619	584.60
135.00	4.678	4.862	9.540	656.33	7.752	631.57
140.00	4.857	4.967	9.824	695.42	7.883	679.99
145.00	5.033	5.070	10.103	735.16	8.011	729.81
150.00	5.207	5.170	10.377	775.52	8.135	781.01
155.00	5.378	5.268	10.646	816.50	8.254	833.57
160.00	5.547	5.363	10.909	858.06	8.368	887.46
165.00	5.713	5.456	11.169	900.17	8.477	942.66
170.00	5.877	5.546	11.423	942.82	8.580	999.14
175.00	6.039	5.634	11.673	985.97	8.679	1056.9
180.00	6.199	5.720	11.919	1029.6	8.774	1115.9
185.00	6.357	5.804	12.161	1073.7	8.865	1176.1
190.00	6.513	5.886	12.399	1118.3	8.955	1237.5
195.00	6.667	5.965	12.632	1163.2	9.042	1300.0
200.00	6.819	6.043	12.862	1208.7	9.126	1363.8
205.00	6.969	6.120	13.089	1254.5	9.209	1428.7
210.00	7.117	6.194	13.311	1300.7	9.289	1494.7
215.00	7.264	6.267	13.531	1347.4	9.366	1561.8
220.00	7.409	6.338	13.747	1394.4	9.443	1630.0
225.00	7.552	6.408	13.960	1441.8	9.519	1699.2
230.00	7.694	6.477	14.170	1489.6	9.597	1769.6
235.00	7.834	6.544	14.378	1537.8	9.677	1840.9
240.00	7.972	6.610	14.582	1586.4	9.758	1913.3
245.00	8.109	6.675	14.784	1635.4	9.842	1986.8
250.00	8.245	6.739	14.984	1684.8	9.924	2061.2
255.00	8.379	6.802	15.181	1734.6	10.004	2136.6
260.00	8.511	6.865	15.376	1784.8	10.079	2213.0
265.00	8.643	6.926	15.569	1835.4	10.149	2290.3
270.00	8.773	6.986	15.759	1886.3	10.213	2368.7
273.15	8.854	7.024	15.878	1918.5	10.250	2418.5
275.00	8.902	7.046	15.947	1937.5	10.271	2447.9
280.00	9.029	7.104	16.133	1989.0	10.326	2528.1
285.00	9.155	7.161	16.316	2040.8	10.380	2609.3
290.00	9.280	7.217	16.497	2092.8	10.435	2691.3
295.00	9.404	7.272	16.676	2145.1	10.492	2774.2
298.15	9.482	7.306	16.787	2178.2	10.531	2826.9
300.00	9.527	7.326	16.853	2197.7	10.555	2858.0

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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. Absolute Electrical Measurements.

Metrology. Photometry and Colorimetry. Refractometry. Photographic Research. Length. Engineering Metrology. Mass and Volume.

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. 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. Far Ultraviolet Physics. Solid State Physics. Electron Physics. Atomic Physics. Plasma Spectroscopy.

Instrumentation. Engineering Electronics. Electron Devices. Electronic Instrumentation. Mechanical Instruments. Basic Instrumentation.

Physical Chemistry. Thermochemistry. Surface Chemistry. Organic Chemistry. Molecular Spectroscopy. Elementary Processes. Mass Spectrometry. Photochemistry and Radiation Chemistry.

Office of Weights and Measures.

BOULDER, COLO.

CRYOGENIC ENGINEERING LABORATORY

Cryogenic Processes. Cryogenic Properties of Solids. Cryogenic Technical Services. Properties of Cryogenic Fluids.

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.

Troposphere and Space Telecommunications. Data Reduction Instrumentation. Radio Noise. Tropospheric Measurements. Tropospheric Analysis. Spectrum Utilization Research. Radio-Meteorology. Lower Atmosphere Physics.

Radio Systems. Applied Electromagnetic Theory. High Frequency and Very High Frequency Research. Frequency Utilization. Modulation Research. Antenna Research. Radiodetermination.

Upper Atmosphere and Space Physics. Upper Atmosphere and Plasma Physics. High Latitude Ionosphere Physics. Ionosphere and Exosphere Scatter. Airglow and Aurora. Ionospheric Radio Astronomy.

RADIO STANDARDS LABORATORY

Radio Standards Physics. Frequency and Time Disseminations. Radio and Microwave Materials. Atomic Frequency and Time-Interval Standards. Radio Plasma. Microwave Physics.

Radio Standards Engineering. High Frequency Electrical Standards. High Frequency Calibration Services. High Frequency Impedance Standards. Microwave Calibration Services. Microwave Circuit Standards. Low Frequency Calibration Services.

Joint Institute for Laboratory Astrophysics - NBS Group (Univ. of Colo.).