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THERMODYNAMICS OF CERTAIN REFRACTORY COMPOUNDS

Part II. Continued Theoretical and Experimental Studies on an Extended List

Second Quarterly Progress Report
1 September to 30 November 1962

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ABSTRACT

A compilation of the thermodynamic properties of refractory borides, carbides, nitrides, and oxides of some 31 elements is the objective of this study. This report presents the data accumulated in the past 3 months of literature review and computations, using the best available data.

Review of the literature has uncovered over 2500 references, and this survey is being continued.

In this report, several tables for elements and compounds not previously reported have been presented, and the experimental spectroscopic studies of the vapor of boron oxide and hydroxide have been discussed.

ACKNOWLEDGMENTS

In a project of this nature, the help and cooperation of many individuals here and elsewhere are gratefully acknowledged.

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I. INTRODUCTION

In the First Quarterly Progress Report of this project, the general aims and scope have been discussed. These aims include the preparation of thermodynamic data tables for the borides, carbides, nitrides, and oxides of some 31 elements. Three primary phases of this project are recognized to accomplish the goals set forth. They are as follows: (Phase I) a review of the literature, (Phase II) analyses and computations of the pertinent thermodynamic data, and (Phase III) an experimental spectroscopic program to determine thermodynamic quantities for systems of interest to the project.

II. REVIEW OF LITERATURE AND COMPILATION OF AVAILABLE DATA

A. REVIEW OF LITERATURE

The method for reviewing thermodynamic literature generally follows the pattern outlined in section II of the First Quarterly Progress Report. Continued emphasis is placed on the Chemical Abstracts and Nuclear Science Abstracts. However, other sources listed in the First Quarterly are also being utilized.

In the current project, a total of about 2500 references have been obtained on the primary ASM cards. These cards are then processed onto bibliographic IBM cards and property IBM cards. Of the 2500 references, approximately 1500 have been completely processed while the remaining 1000 are partially processed.

B. CLASSIFIED LITERATURE SOURCES

Review of the classified AEC literature on file at the AEC library in New York City was extended. As before, a small amount of thermodynamic data was found which had not been published in the open literature. This survey of the available documents in New York should be completed relatively soon. To inspect documents not held by them, it might be necessary to consult the AEC library at Oak Ridge.

C. PROBLEM OF COMPATIBILITY OF RAD TABLES WITH JANAF TABLES

In the First Quarterly Progress Report, several aspects of the problem of compatibility of RAD thermodynamic tables and JANAF tables were discussed. As a result of discussions with D. R. Stull, it would seem unlikely that any serious discrepancies were occurring between the two tabulations. It was agreed that future tables would be prepared so that each group would be informed of the work done in areas of mutual interest.

In view of the desirability of issuing tables which can be used interchangeably with the JANAF tables, an effort has been made to develop a format for the tables (front page and back) which follows the normal JANAF format. Copies of the basic Avco format sheets are included (see figures II-1 to II-5). It is anticipated that future reports will use these formats exclusively although the present report still follows the pattern of earlier reports. The format sheets illustrated follow the general JANAF scheme; however, provisions for uncertainty estimates and a separate tabulation of references are retained.

D. PHYSICAL CONSTANTS

Another problem concerned with table compatibility is that of suitable choice of physical constants. As discussed in the First Quarterly Progress

Report, RAD tables use the same constants, including the old molecular weight scale, as have been used in the first year's work on this contract. This also follows the pattern used by JANAF.

In connection with the new constants, the latest available data appear to be that of Cohen and others.[1] This work leads to a value for the gas constant of R = 1.98717 cal/mole °K instead of the 1.98726 cal/mole °K now being used. Thus, the change in gas constant is quite small. It is possible that this number may be revised again since Cohen and co-workers[2] expect to be able to "submit a reasonably reliable adjustment of the physical constants to the National Research Council Committee on Fundamental Constants within the next several months." It appears likely that further small changes may be expected.

In view of these uncertainties and the fact that the corrections will be very small, it still appears best to continue the policy outlined earlier; namely, to use the "old" constants of the previous project until a definite set of "new" constants is obtained.

REFERENCES FOR SECTION IIC

1. Cohen, E. R., J. W. M. DuMond, and A. G. McNish, Most Probable Values of the Physical Constants, Am. Phys. Soc. Mtg., Washington, D. C. (24 April 1962).

2. Cohen, E. R., Private Communication with H. L. Schick (8 November 1962).

BASIC DATA FORMAT FOR REFERENCE STATE ELEMENTS

______________ (   ) (REFERENCE STATE) gfw = __________
(Name) *(Formula)*

0 °K to __________ °K Crystal

______ °K to __________ °K Liquid

______ °K to __________ °K Ideal Monatomic Gas

$\Delta H^{\circ}_{f0} = 0$

$\Delta H^{\circ}_{f298.15} \doteq 0$

$\Delta H^{\circ}_{s\,298.15}$ = __________ Kcal.gfw^{-1}

$S^{\circ}_{298.15}$ = __________ cal.deg^{-1}.gfw^{-1}

T_t = __________ °K

ΔH_t = __________ Kcal.gfw^{-1}

T_m = __________ °K

ΔH_m = __________ Kcal.gfw^{-1}

T_b = __________ °K

ΔH_v = __________ Kcal.gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_0$ = ________ Kcal.gfw^{-1}

C°_p = __________ l.deg^{-1}.gfw^{-1} ________ °K $\leq T \leq$ ________ °K

____

____
(Statement of Structure)

Summary of Uncertainty Estimates *(Optional: if data avail.)*

	cal/°K gfw			Kcal/gfw			
T,°K	C°_p	S°_T	$-(F^{\circ}_T - H^{\circ}_{298})/T$	$H^{\circ}_T - H^{\circ}_{298}$	ΔH°_f	ΔF°_f	log K_p

Heat of Formation

____

Heat Capacity and Entropy

____

Melting

____

Vaporization

____

References

____

Figure II-1

BASIC DATA FORMAT FOR MONATOMIC GASES

______________ ( ) (IDEAL GAS) gfw = ______________

(Name) *(Formula)*

ΔH°_{f0} = ______________ Kcal.gfw^{-1}

$\Delta H^{\circ}_{f298.15}$ = ______________ Kcal.gfw^{-1}

Ground State Configuration ______________

$S^{\circ}_{298.15}$ = ______________ cal.deg^{-1}.gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_{0}$ ______________ Kcal.gfw^{-1}

Electronic levels and multiplicities

____

(Statement of Source of data)

____

____

____

Summary of Uncertainty Estimates *(Optional: if data avail.)*

	cal/°K gfw			Kcal/gfw			
T,°K	C°_{p}	S°_{T}	$-(F^{\circ}_{T} - H^{\circ}_{298})/T$	$H^{\circ}_{T} - H^{\circ}_{298}$	ΔH°_{f}	ΔF°_{f}	log K_p

Heat of Formation

____

____

____

Heat Capacity and Entropy

____

____

____

References

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____

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Figure II-2

BASIC DATA FORMAT FOR CONDENSED PHASE COMPOUNDS

__________ (   ) (CONDENSED PHASE) gfw = __________
(Name) *(Formula)*

$\Delta H^{\circ}_{f298.15}$ = __________ Kcal.gfw^{-1}

$S^{\circ}_{298.15}$ = __________ cal.deg.$^{-1}$gfw^{-1}

T_t = __________ °K

ΔH_t = __________ Kcal.gfw^{-1}

T_m = __________ °K

ΔH_m = __________ Kcal.gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_0$ __________ Kcal.gfw^{-1}

C°_p = __________ cal.deg^{-1}.gfw^{-1} ______ °K ≤ T ≤ ______ °K

____

____

____
(Statement of Structure)

Summary of Uncertainty Estimates *(Optional: if data avail.)*

	cal/°K gfw			Kcal/gfw			
T,°K	C°_p	S°_T	$-(F^{\circ}_T - H^{\circ}_{298})/T$	$H^{\circ}_T - H^{\circ}_{298}$	ΔH°_f	ΔF°_f	log K_p

Heat of Formation

____

____

____

Heat Capacity and Entropy

____

____

____

Melting and Vaporization

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____

____

References

____

____

____

Figure II-3

BASIC DATA FORMAT FOR DIATOMIC MOLECULAR GASES

______________ (   )   (IDEAL GAS)   gfw = ____________
(Name)   *(Formula)*

ΔH°_{f0} = ____________ Kcal.gfw^{-1} $\Delta H^{\circ}_{f298.15}$ = ____________ Kcal.gfw^{-1}

Ground State Configuration ____________ $S^{\circ}_{298.15}$ = ____________ cal.deg^{-1}.gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_{0}$ = ____________ Kcal.gfw^{-1}

		cm^{-1}							
State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$

Summary of Uncertainty Estimates *(Optional: if data avail.)*

	cal/°K gfw			Kcal/gfw			
T,°K	C°_p	S°_T	$-(F^{\circ}_T - H^{\circ}_{298})/T$	$H_T - H_{298}$	ΔH°_f	ΔF°_f	log K_p

Heat of Formation

____

____

____

Heat Capacity and Entropy

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References

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Figure II-4

________________ ( ) (IDEAL GAS) gfw = ________
(Name) *(Formula)*

ΔH°_{f0} = ________________ Kcal.gfw^{-1} $\Delta H^{\circ}_{f298.15}$ = ________________ Kcal.gfw^{-1}

Point Group ________ $S^{\circ}_{298.15}$ = ________________ cal.deg.$^{-1}$gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_{0}$ ________________ Kcal.gfw^{-1}

Vibrational levels and multiplicities

ω, cm^{-1} ω, cm^{-1}

________ ( ) ________ ( ) *(Note: multiplicities*

________ ( ) ________ ( ) *inserted in ( ))*

Bond lengths and angles:

________________ distance = ________ Å ________________ distance = ________ Å

________________ Angle = ________

Product of moments of inertia: $I_A I_B I_C$ = ________ g^3.cm^6 σ = ________

Summary of Uncertainty Estimates *(Optional: if data avail.)*

	cal/°K gfw			Kcal/gfw			
T,°K	C°_{p}	S°_{T}	$-(F^{\circ}_{T} - H^{\circ}_{298})/T$	$H^{\circ}_{T} - H^{\circ}_{298}$	ΔH°_{f}	ΔF°_{f}	log K_p

Heat of Formation

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Heat Capacity and Entropy

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References

____

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Figure II-5

III. CALCULATIONAL PROCEDURES

A. NEW COMPUTATIONAL PROGRAMS

Because of the fact that much existing experimental data are not reported in a form suitable for direct inclusion in the RAD tables, it has been desirable to develop new computational programs.

Program No. 1316 has been developed to fit, by a least-squares technique, an empirical equation to experimentally observed heat contents. The forms of the equation are

$$H_T - H_{Tref} = K_a + A_a T + \frac{B_a}{2} T^2 - C_a T^{-1} \quad , \qquad \text{(IIIA-1)}$$

$$C_p = A_a + B_a T + C_a T^{-2} \quad , \qquad \text{(IIIA-2)}$$

and

$$H_T - H_{Tref} = K_b + A_b T + \frac{B_b}{2} T^2 + \frac{C_b}{3} T^3 \quad , \qquad \text{(IIIA-3)}$$

$$C_p = A_b + B_b T + C_b T^2 \quad . \qquad \text{(IIIA-4)}$$

By observing the deviations and the sums of the deviations squared, it is possible to make a choice of the most appropriate equations from the two groups shown above.

Another program with which it is intended to derive heat-of-formation data from equilibrium pressure data is nearing completion. This program utilizes partial pressure data and free-energy functions of the pertinent species to obtain the heat of reaction at 298.15°K. This program may be used to obtain vapor-pressure equilibria or more complex equilibria.

A third computer program is employed to smooth "raw" experimental heat-capacity data before incorporation in a table.

A modification of the polyatomic gas program has been developed which will permit calculation of the product of the principal moments of inertia of the molecule from the cartesian coordinates of its constituent atoms. Thus, a separate hand calculation, as has been required earlier, is avoided.

B. THE DIVERGENCE PROBLEM

There is an ever-present problem of divergence at high temperatures in the formulas for the thermodynamic functions from statistical mechanics, when one uses them with the usual spectroscopic expression for the energy of a diatomic molecule including anharmonic and vibration-rotation interaction terms. With a potential function such as the Morse function ordinarily used to represent chemical bonding, there results an infinite number of energy states converging to an upper energy limit located at zero potential. The partition function is therefore infinite under all conditions. The energy expression used by spectroscopists consists of only the first few terms of an infinite power series in the rotational and vibrational quantum numbers, and it should be used only for energies far below the aforementioned convergence limit. Nevertheless, some of these terms, involving the highest powers of the quantum numbers in the expression, are negative and result in positive exponential terms in the partition function, which diverge if carried to large quantum numbers.

In practice, however, one can obtain sufficiently good values for the partition function and derived thermodynamic functions at low temperatures by cutting the series off after a few terms. This approximation becomes progressively worse as the temperature is raised and the divergence increases.

The degree of divergence depends upon the depth of the potential well; and in cases of low binding energy, divergence can be serious at temperatures far below the upper limit of the calculations; namely, 6000°K.

It is very difficult to specify the extent of error introduced by this divergence, and arbitrary cutoff procedures have often been adopted for the divergent terms. However, one is never sure that these cutoff procedures result in better values of the functions at any particular temperature. At low temperatures, the anharmonic, and other, correction terms are unimportant; at intermediate temperatures, they contribute significantly and with sufficient accuracy to be fully retained; and at very high temperatures, one must resort to the uncoupled harmonic oscillator approximation or to an entirely different approach involving cluster integrals.

For the present compilation, the anharmonic, etc., corrections have been fully retained to make low- and intermediate-temperature values of the thermodynamic functions as accurate as possible. Therefore, some inaccuracy undoubtedly exists at the highest temperatures due to the divergence problem; however, it is felt that the values are no worse than those which may have been obtained by neglect of the correction terms or arbitrary cutoff procedures. A concentrated effort has been made to recognize unusual cases where the divergence problem is prohibitively severe below 6000°K.

IV. DATA REVIEWS AND COMPUTATION SUMMARIES FOR INDIVIDUAL ELEMENTS AND COMPOUNDS

A. ELEMENTS

1. Cerium

a. Crystal Structure, Transition Points, and Melting Point

The description of the allotropy of elemental cerium near room temperature and below was found to be complicated by slow rates of the transformations, and hence, by the occurrence of metastable phases. In this range of temperature, two or more modifications might be observed simultaneously in proportions and over temperature ranges which would depend on the thermal and mechanical history of the metal as well as on the presence of small amounts of impurities. McHargue and Yakel[1] recently studied the conditions under which the various allotropic modifications appeared, and their article could be consulted for references to earlier work on the subject.

In general, however, a face-centered cubic form, γ – Ce,* has been considered to be thermodynamically stable between 1003° and about 260°K.[1,2] Crystallographic data for this phase have been given by Spedding, Daane, and Hermann.[3] Between about 260° and about 150°K, the stable form has usually been considered to be hexagonal close-packed β–Ce[1,2] although Dialer and Rothe[4] have reported both β–Ce and γ–Ce to be face-centered cubic.

To complicate the picture still further, Weiner and Raynor[5] were unable to produce a transformation from γ–Ce to β–Ce, and they observed a possible additional face-centered cubic phase. This latter phase, designated by them as γ'–Ce, was observed after annealing γ–Ce for long periods of time above 500°C followed by slow cooling. It was stated, however, that the phase might have been due to small amounts of hydrogen in their sample.

Pure β–Ce had never been reported. Crystallographic data for β–Ce was given by McHargue, Yakel, and Jetter[6] and by McHargue and Yakel.[1] Commercial cerium had been considered to contain sufficient calcium and magnesium to inhibit the formation of γ–Ce from β–Ce.[7]

Below about 150°K, a dense, or "collapsed," face-centered cubic phase, α–Ce, had been considered to be the stable form.[1,2] It had been suggested that the appearance of α–Ce would mark the movement of the one

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*Various authors have adopted different symbols to designate the allotropic modifications of cerium.

4f electron in cerium to the conduction band.[8, 9] This interpretation was consistent with the neutron diffraction studies on metallic cerium by Wilkinson and others.[10] Crystallographic data for α–Ce were given by Lawson and Tang,[8] and by Schuch and Sturdivant.[11] High-pressure studies on cerium[12-16] showed a high-pressure, room-temperature, face-centered cubic phase to be identical with α–Ce. Results of the high-pressure studies were used to arrive at an estimate of S°_{298} for cerium.

Cerium had been reported to exhibit a further heat-capacity anomaly at 12.5 °K.[17, 18] An anomaly at that temperature was also detected in susceptibility measurements.[19] Lock suggested that this anomaly was due to antiferromagnetic ordering, presumably in γ–Ce. Parkinson, Simon, and Spedding[17] made an alternate suggestion that this behavior was due to excitation of electrons between energy levels produced by stark splitting of the ground state. Parkinson and Roberts[18] concluded that the anomaly would occur if 4f electrons were present in the metal; i.e., in β– or γ–Ce. Wilkinson and others,[10] from their neutron diffraction studies, concluded that the anomaly at 12.5 °K was due to antiferromagnetic ordering, and that it occurred in hexagonal close-packed β–Ce. It might be added that it would be possible to study virtually pure α–Ce (i.e., in the absence of significant amounts of γ–Ce) and establish some features of an α–γ transition well below the temperature at which γ–Ce would be believed to be thermodynamically stable.

Cerium containing a mixture of phases at room temperature had been reported to become single-phased γ–Ce when heated to about 420 °K.[1] At 1003° ± 5 °K,[20, 21] γ–Ce had been reported to transform rapidly and reversibly to body-centered cubic δ–Ce;[20] i.e., the stable form at temperatures up to the melting point. Prior to the electrical resistivity measurements[21] which established the γ–δ transition temperature as 1003 °K, thermal analysis studies gave this transition as 1027 °K.[23] Heat-content measurements on δ–Ce at 1016 °K by Spedding, McKeown, and Daane[23] supported the lower transition temperature. This transition temperature should be accepted in preference to the pair of high-temperature transition temperatures tabulated by NBS Circular 500[24] from the work of Jaeger and Rosenbohm,[25] and that of Jaeger, Bottema, and Rosenbohm.[26, 27] Crystallographic data for δ–Ce were given by Spedding, Hanak, and Daane.[20]

b. Thermodynamic Properties

1) Heats of transition and fusion

The heat of the γ–δ transition in cerium was measured by Spedding, McKeown, and Daane[23] and found to be 700 ± 8 cal/gfw at 1003 °K. This gave an entropy of transition of 0.698 ± 0.008 e.u./gfw. They also found the heat of fusion of cerium to be 1238 ± 4 cal/gfw at 1077°K; this corresponded to an entropy of fusion of 1.149 ± 0.004 e.u./gfw. Thus, the entropy of the f.c.c.-b.c.c. transition plus the entropy of fusion were altogether 1.847 ± 0.012 e.u./gfw.

2) Entropy and heat content at 298.15°K

The low-temperature (1.5° to 200°K) heat capacity of cerium was measured by Parkinson, Simon, and Spedding,[17] Simon and Ruhemann,[28] and Parkinson and Roberts.[18] Parkinson, Simon, and Spedding[17] made measurements on two samples of cerium. One sample was stated to contain only γ-Ce at room temperature although its structure at the various measurement temperatures was unknown and was doubtless complicated. A second sample contained a mixture of β-Ce and γ-Ce. Kelley and King[29] adopted the heat-capacity results obtained on the first sample and extrapolated them to obtain a value of 7.02 cal/°K gfw at 298.15°K. They reported S^o_{298} to be 16.6 ± 1.0 e.u./gfw. This was the value of S^o_{298} tabulated by Parkinson, Simon, and Spedding[17] for γ-Ce from their heat-capacity measurements after adding 0.35 e.u./gfw to correct for the effect of the α-Ce present on the entropy of the transition at 12.5°K. The results of Parkinson and Roberts,[18] from studies on γ-Ce between 1.5° and 20°K, suggested that a further correction of 0.16 e.u./gfw should be made to give a true value of 16.8 e.u./gfw for the S^o_{298} of γ-Ce.

There was considerable uncertainty as to the phase composition of the cerium during most of the above-described measurements. The heat capacity of 6.90 cal/°K gfw at 200°K was considerably larger than the value of 6.440 cal/°K gfw at 298.15°K from the high-temperature measurements of Spedding, McKeown, and Daane.[23] Therefore, S^o_{298} was herein estimated as the sum of a lattice vibration contribution from an adopted Debye characteristic temperature, a contribution from the electronic heat capacity and $C^o_p - C_v$, and a contribution from an α-γ transition taken to occur at 150°K.

The Debye characteristic temperature of γ-Ce from the results of Parkinson, Simon, and Spedding,[17] obtained from studies at temperatures between 20° and 40°K, was 115 ± 2°K. This value of θ_D was supported by the results of measurements by Parkinson and Roberts[18] on γ-Ce near 20°K. It was used for the estimates of lattice vibration contributions to S^o_{298} and $H^o_{298} - H^o_0$. These contributions were 13.650 e.u./gfw and 1.534 kcal/gfw, respectively. The estimated lattice specific heat at 298.15°K was 5.918

cal/°K gfw. The combined contribution of electronic specific heat and $C_p^o - C_v$ was estimated to be proportional to the absolute temperature and to be equal, at 298.15°K, to the difference between the adopted C_p^o and the lattice specific heat, or 0.520 cal/°K gfw. The resulting contributions to S_{298}^o and $H_{298}^o - H_0^o$ were 0.520 e.u./gfw and 0.078 kcal/gfw, respectively.

The high-pressure studies of Poniatovskii,[13] Likhter, Riabinin, and Vereshchagin,[16] Herman and Swenson,[14] and Beecroft and Swenson[15] showed that the α–γ phase transformation varied linearly with pressure and that $dP/dT = 43 \pm 2$ atm/°K. The data could be extrapolated to a transition temperature of 150° ± 20°K at 1 atm pressure. From X-ray measurements, Lawson and Tang[8] and Schuch and Sturdivant[11] reported $\Delta V/V_o$ for this transition to be 0.165 at atmospheric pressure. The molar volume of cerium was taken to be 20.2 cm^3. The Clausius-Clapeyron equation was used with these data to calculate an entropy of transition of 3.470 e.u./gfw and a heat of transition of 0.521 kcal/gfw at 150°K. Thus, the adopted value of S_{298}^o became 17.640 e.u./gfw and that of $H_{298}^o - H_0^o$ was 2.133 kcal/gfw. An uncertainty of ± 0.800 e.u./gfw was assigned to the entropy.

Jennings[30] used a similar procedure to estimate S_{298}^o to be 18.12 e.u./gfw, a value which was adopted by Spedding, McKeown, and Daane.[23] Hultgren and others[31] similarly estimated S_{298}^o to be 15.3 ± 2 e.u./gfw. From a comparison of the values of S_{298}^o for the various rare earths for which there were the most reliable experimental data,[29] a value of 18.0 e.u./gfw appeared to be reasonable.

3) High-temperature heat content

The high-temperature heat-content measurements of Spedding, McKeown, and Daane[23] superseded the earlier measurements of Jaeger and Rosenbohm,[25] and those of Jaeger, Bottema, and Rosenbohm,[26,27] on which the compilations of Kelley[32] and Stull and Sinke[33] were based. The results of Spedding, McKeown, and Daane (with C_p^o in cal/°K gfw)[23] could be represented over the temperature range of 298° to 1400°K by the following equations:

$$C_p^o\ (\gamma) = 5.649 + 2.300 \times 10^{-3}\,T + 11.862 \times 10^{-7}\,T^2\ , \qquad \text{(IVA1-1)}$$

$$C_p^o\ (\delta) = 9.047\ \text{cal/}^\circ\text{K gfw.} \qquad \text{(IVA1-2)}$$

$$C_p^o \text{ (liq.)} = 9.345 \text{ cal/}^oK \text{ gfw.} \qquad \text{(IVA1-3)}$$

$$\Delta H\ (\gamma - \delta)_{1003^o} = 0.700 \pm 0.008 \text{ kcal/gfw.} \qquad \text{(IVA1-4)}$$

$$\Delta H\ (\delta - \text{liq.})_{1077^o} = 1.238 \pm 0.004 \text{ kcal/gfw.} \qquad \text{(IVA1-5)}$$

The above value of the heat capacity of liquid cerium was adopted for use up to the boiling point.

4) Ideal monatomic gas

It was not possible to calculate the ideal monatomic gas thermodynamic functions of cerium from its energy levels as the latter had not been tabulated. For purposes of the present compilation, the energy levels of cerium gas were assumed to be identical to those of lanthanum as listed by Moore.[34]

5) Standard heat of formation of the gas and the boiling point

The vapor pressure of cerium was measured by Brewer,[35] Ahmann,[36] Daane and Spedding,[37] and Gilles and Jackson.[38] The data of the last authors were not available. However, Spedding and Daane[2] reported that the heat of vaporization from the data of Gilles and Jackson[38] was somewhat higher than the value reported by Ahmann,[36] and Daane and Spedding.[37] Ahmann[36] represented his data by the equation

$$\log P_{mm} = \frac{-23400 \pm 440}{T} + 11.58 \pm 0.27 \quad , \qquad \text{(IVA1-6)}$$

and Daane and Spedding[37] represented their data by the equation

$$\log P_{mm} = \frac{-20304 \pm 81}{T} + 8.3062 \pm 0.0447 \quad . \qquad \text{(IVA1-7)}$$

The results of the first three authors[35-37] were in wide disagreement but bracketed ΔH_s^o at 298.15 °K between 80 and 111 kcal/gfw. The agreement between calculations of ΔH_{f298}^o by Second and Third Law methods was also very poor. However, because of the assumption made in calculating the thermodynamic functions for monatomic cerium gas, this comparison should not be pushed too far. Spedding and Daane[2] recommended a value of 95 kcal/gfw for ΔH°_{f298} ,and the same value could be estimated from a comparison of that quantity for other rare-earth metals.[2,39,40] This value was adopted herein, and an uncertainty of ± 2.500 kcal/gfw was assigned to it.

The normal boiling point of cerium was calculated to be 4270.73° ± 490°K. This boiling point was considerably higher than the value of 3200°K given by Stull and Sinke[33] and of 3742°K given by Hultgren and others.[31] The increase in the normal boiling point was due to the attempt to include a contribution from the energy levels of cerium gas to its thermodynamic functions and/or the adoption of a larger ΔH_s value at 298.15°K.

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2. Manganese

a. Crystal Structure, Transition Points, and Melting Point

Elemental manganese had been reported to have four crystalline modifications for which the following transformation temperatures in °K were selected:

$$\alpha \xleftrightarrow{990^\circ \pm 15^\circ} \beta \xleftrightarrow{1374^\circ \pm 10^\circ} \gamma \xleftrightarrow{1410^\circ \pm 5^\circ} \delta \quad .$$

Sully[1] summarized most of the experimental data concerning transformation temperatures for manganese. Additional data were obtained by Dean and others,[2] and Armstrong and Grayson-Smith.[3] The adopted β–γ and γ–δ transformation temperatures were taken from the manganese heat-content measurements of Naylor.[4, 5] The temperature given by Naylor for the sluggish α–β transformation, 1000°K, was an upper limit. An average of his α–β transformation temperatures on heating and cooling through the transition was 980°K. The heat-capacity measurements of Armstrong and Grayson-Smith[3] revealed the α–β transition temperature to be 990°K.

α–Mn was found to have a body-centered cubic structure, type A1;[6-11] the structure of β–Mn was found to be a primitive cubic, A13 type;[7,9-13] the structure of γ–Mn (in the temperature range of thermodynamic stability) was found to be the face-centered cubic, A1 type;[13, 14] and δ–Mn was found to have a body-centered cubic, A2-type structure.[13] γ–Mn had been obtained at room temperature as a face-centered tetragonal crystal by electrodeposition of the metal.[4, 15, 16] However, this form could not be retained completely by quenching from a temperature at which it was stable. The tetragonal structure could be stabilized at low temperatures in manganese alloys.[1] The rate of transformation of metastable γ–Mn to α–Mn at various temperatures was studied by Potter, Lukens, and Huber.[16] At 298°K, the half-time of the γ–α transformation was 238 hours; at 373°K, the half-time was 15 minutes; and at 433°K, it was 7.7 seconds. The transformation temperature between the tetragonal and face-centered cubic structures of γ–Mn as a function of the manganese content of manganese-copper alloys was studied by Basinski and Christian.[17]

Sully[1] reviewed manganese melting-point determinations and selected a temperature of 1517° ± 3°K for the melting point, which was adopted for the present compilation. The given uncertainty covered six of eight determinations reported since 1927 as listed by Sully.[1] Moser, Raub, and Vincke[18] reported a melting point of 1520°K.

b. Thermodynamic Properties

1) Heats of transition and fusion

The heats of transition adopted were those calculated from the analytical representations of the high-temperature heat-content measurements of Naylor[4, 5] at the following adopted transition temperatures:

Transition	Temperature	Heat of Transition
	°K	cal/gfw
$\alpha-\beta$	990	531 ± 80
$\beta-\gamma$	1374	549 ± 80
$\gamma-\delta$	1410	436 ± 60

Other relatively reliable values for the heat of the α–β transformation were 615 cal/gfw at 1012°K reported by Southard and Shomate,[19] and 450 cal/gfw reported by Armstrong and Grayson-Smith.[3] There were no other reliable measurements of the heats of the β–γ and γ–δ transformations.

The heat of fusion of manganese given by Kelley, Naylor, and Shomate,[5] 3500 cal/gfw, was adopted herein. This value was based on a heat of fusion of 3450 cal/gfw at 1493°K reported by Umino.[20] Kelley[21] obtained a value of 3650 cal/gfw from analysis of phase data for several manganese alloys. Kubaschewski[22] selected a lower heat of fusion equal to 3200 ± 600 cal/gfw from the same sources on the assumption that the thermal effects involved included a contribution from the then unknown γ–δ transformation. The problem of finding a suitable container material for liquid manganese apparently complicated the experimental measurement of the heat of fusion.

2) Low-temperature heat capacity

a) α–Mn

The low-temperature heat capacity of α–Mn has been measured by Gaumer,[23] Wolcott,[24] Guthrie, Friedberg, and Goldman,[25] Booth, Hoare, and Murphy,[26] Elson, Grayson-Smith, and Wilhelm,[27] Armstrong and Grayson-Smith,[28] Kelley,[29] and

Shomate.[30] There has been considerable interest in the heat capacity of manganese at very low temperatures since the metal has one of the highest electronic specific heats known.

Kelley and King[31] reported S°_{298} for α–Mn to be 7.640 ± 0.040 e.u./gfw from the measurements of Booth, Hoare, and Murphy[26] and Shomate.[30] This value was adopted herein. The results of Wolcott,[24] Elson, Grayson-Smith, and Wilhelm,[27] and Armstrong and Grayson-Smith[28] agreed well with each other but were some 25 percent higher than those of Guthrie, Friedberg, and Goldman,[25] and Booth, Hoare, and Murphy.[26] S°_{298} for α–Mn was calculated by Stull and Sinke[32] and by Hultgren and others,[33] to be 7.650 e.u./gfw.

b) β–Mn

The low-temperature heat capacity of metastable β–Mn (produced by quenching β–Mn at 1393°K in water) was measured by Booth, Hoare, and Murphy.[26]

c) γ–Mn

Shomate[5,30] measured the low-temperature heat capacity of metastable γ–Mn (produced by electrolytic decomposition) from 53° to 297°K. From these data, Kelley and King[31] calculated an S°_{298} value of 7.720 ± 0.040 e.u./gfw for γ–Mn, of which 0.49 e.u./gfw was from an extrapolation below 53°K.

3) High-temperature heat content

The high-temperature heat content or heat capacity of manganese was measured by Armstrong and Grayson-Smith,[3] Laemmel,[34] Naylor,[4, 5] Southard and Shomate,[19] Stücker,[35] Umino,[20] and Wüst, Meuthen, and Durrer.[36]

The data of Naylor were adopted, with the exception of the noted modification of the α–β transition temperature, and extrapolated to the melting point. The following heat-capacity equations (in cal/°K gfw) were used over the temperature range of 298° to 1517°K together with the heats of transition given above:

$$C^{\circ}_{p}\ (\alpha\text{–Mn}) = 5.704 + 3.380 \times 10^{-3}\,T - 0.375 \times 10^{5}\,T^{-2} \qquad \text{(IVA2-1)}$$

$$C^{\circ}_{p}\ (\beta\text{–Mn}) = 8.330 + 0.660 \times 10^{-3}\,T \qquad \text{(IVA2-2)}$$

$$C_p^\circ\ (\gamma\text{–Mn}) = 10.700 \qquad \text{(IVA2-3)}$$

$$C_p^\circ\ (\delta\text{–Mn}) = 11.300\ . \qquad \text{(IVA2-4)}$$

The agreement between the results of the various authors was not good. Other measurements on α–Mn with metal of known high purity by Armstrong and Grayson-Smith,[3] and Southard and Shomate[19] gave heat capacities 1 to 3 percent lower than the adopted data. However, Naylor's data were preferred as they joined well with the low-temperature heat-capacity measurements and formed part of an internally consistent set of data for all crystalline modifications.

Armstrong and Grayson-Smith measured the heat capacity of β–Mn over a narrow range of temperatures less than 100° above the α–β transition temperature. Their data showed a greater temperature dependence of the heat capacity of β–Mn than that found by Naylor although the two sources were in excellent agreement at 1073°K. Southard and Shomate's results for β–Mn were only in fair agreement with those of Naylor. Naylor's results were the only reliable ones for γ– and δ–Mn. He also derived a heat-capacity equation for γ–Mn in the temperature range of 298° to 1347°K, where the latter modification was metastable. Recalculation of this equation with the thermodynamic functions for α–Mn from this compilation yielded equation (IVA2-5) for C_p° in cal/°K gfw over the temperature range of 298° to 1374°K.

$$C_p^\circ\ (\gamma\text{–Mn}) = 5.997 + 3.625 \times 10^{-3}T - 0.434 \times 10^{5}T^{-2}\ . \qquad \text{(IVA2-5)}$$

An extrapolation of this equation to the range of stability of γ–Mn gave an average heat capacity of 11.020 cal/°K gfw as compared with the experimental value of 10.700 cal/°K gfw. Thermodynamic functions of metastable γ–Mn had been given elsewhere;[5, 33, 37] however, they were not included in the present compilation which superseded them.

4) Standard heat of formation of the gas at 298.15°K

The vapor pressure of manganese was measured by Bauer and Brunner,[38] McCabe and Hudson,[39] Butler, McCabe, and Paxton,[40] Evseev and Pozharskaya,[41] and Woolf, Zellars, Foerster, and Morris.[42]

The following heats of formation of the gas in kcal/gfw at 298.15°K were calculated with the Third Law method and vapor-pressure data from the latter sources and thermodynamic functions for manganese from the present compilation:

Source	ΔH°_{f298} of the Gas
Bauer and Brunner[38]	68.150 ± 0.650
McCabe and Hudson[39]	67.110 ± 0.400
Butler, McCabe, and Paxton[40]	67.210 ± 0.250
Woolf *et al*[42]	66.780 ± 0.100

From the last three values, a standard heat of formation of 67.000 ± 0.300 kcal/gfw was selected for Mn as an ideal gas at 298.15°K.

Only a Second Law treatment was possible for the data of Evseev and Pozharskaya. At 298.15°K, a heat of formation of 68.760 kcal/gfw was calculated for the gas with their vapor-pressure equation. However, by neglecting deviating data at one temperature, one can make a new plot giving a heat of formation near the adopted value.

Stull and Sinke[32] reported, from a private communication from Brewer, the heat of formation of the gas to be 66.730 kcal/gfw at 298.15°K.

The normal boiling point and corresponding heat of vaporization were calculated to be 2318.80° ± 50°K and 52.753 ± 2.280 kcal/gfw, respectively.

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3. Platinum

a. Crystal Structure and Melting Point

Elemental platinum was found to have a face-centered cubic, A1-type structure.[1-3] No other allotropic modifications were reported.

A melting point of 2043° ± 3°K was taken from the results of Roeser, Caldwell, and Wensel,[4] Hoffmann and Tingwaldt,[5] and Schofield[6] after correction to the International Temperature Scale of 1948. A melting point of 2033° ± 2°K was also reported later;[7] however, it was not considered as reliable as the earlier value.

b. Thermodynamic Properties

1) Heat of fusion

In the absence of experimental data, an entropy of fusion of 2.300 ± 0.390 e.u./gfw was assumed. This corresponded to a heat of fusion of 4.699 kcal/gfw, to which an uncertainty of ± 0.800 kcal/gfw was assigned.

2) Entropy and heat content at 298.15°K

The low-temperature heat capacity of platinum was measured by Rayne,[8] Ramanathan and Srinivasan,[9] Budworth, Hoare, and Preston,[10] Kok and Keeson,[11] Simon and Zeidler,[12] and Clusius, Losa, and Franzosini.[13] From the data of the last three sources, Kelley and King[14] calculated S°_{298} to be 9.950 ± 0.050 e.u./gfw. The same value was given in the compilation of Clusius, Losa, and Franzosini[13] (calculated from their results by Hultgren and others[15]) and was adopted herein. $H^{\circ}_{298} - H^{\circ}_{0}$ was taken to be 1.372 kcal/gfw from Hultgren and others.[15]

3) High-temperature heat content

The platinum tables in the present compilation were based on the high-temperature heat-content measurements of Jaeger and Rosenbohm,[16] Jaeger, Rosenbohm, and Bottema,[17] and White.[18] Kelley's[19] article may be consulted for references to a number of other measurements.

The heat-capacity results of Jaeger and Rosenbohm[16] were represented(in cal/°K gfw) from 273° to 473°K and 473° to 1873°K, respectively, by the equations

$$C_p^\circ = 5.567 + 2.273 \times 10^{-3}\,T - 0.0942 \times 10^{-5}\,T^2 \quad , \qquad \text{(IVA3-1)}$$

and

$$C_p^\circ = 5.831 + 1.238 \times 10^{-3}\,T \quad . \qquad \text{(IVA3-2)}$$

The results of Jaeger, Rosenbohm, and Bottema[17] were represented in the same units over the temperature range from 273° to 1673°K by the equation

$$C_p^\circ = 5.846 + 1.248 \times 10^{-3}\,T - 3.170 \times 10^{-8}\,T^2 \quad , \qquad \text{(IVA3-3)}$$

and those of White[18] were likewise represented by the equation

$$C_p^\circ = 5.841 + 1.249 \times 10^{-3}\,T \quad . \qquad \text{(IVA3-4)}$$

For the present compilation, the following equations were adopted to join smoothly the low-temperature (298° to 500°K) and high-temperature (500° to 2043°K) data, respectively, in cal/°K gfw:

$$C_p^\circ = 6.028 + 0.969 \times 10^{-3}\,T - \frac{0.1220 \times 10^5}{T^2} \quad , \qquad \text{(IVA3-5)}$$

and

$$C_p^\circ = 5.810 + 1.260 \times 10^{-3}\,T - \frac{0.060 \times 10^5}{T^2} \quad . \qquad \text{(IVA3-6)}$$

The heat capacity of liquid platinum had not been measured and was assumed to be 8.500 cal/°Kgfw to be consistent with the above equations. Kelley[19] assumed it to be 8.300 cal/°Kgfw.

4) Standard heat of formation of the gas at 298.15°K

The vapor pressure of platinum was measured by Jones, Langmuir, and Mackay,[20] Dreger and Margrave,[21] and Hampson and Walker.[22] The data of Jones, Langmuir, and Mackay[20] were corrected to the International Temperature Scale of 1948. The following values for the heat of formation of the gas at 298.15°K were calculated with the Third Law method and the thermodynamic functions for platinum given herein:

Source of Vapor-Pressure Data	ΔH°_{f298}
	kcal/gfw
Jones, Langmuir, and Mackay[20]	134.890 ± 1.100
Dreger and Margrave[21]	135.180 ± 1.200
Hampson and Walker[22]	135.010 ± 0.900

A value of 135.100 ± 0.300 kcal/gfw was adopted for the present compilation.

The normal boiling point was calculated to be 4108.34° ± 95°K, and the associated heat of vaporization was found to be 121.519 ± 5.670 kcal/gfw. These quantities were very little changed from those given by Stull and Sinke.[23]

The ideal monatomic gas properties were taken from the previous calculation on this project.[24]

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4. Rhenium

a. Crystal Structure and Melting Point

Elemental rhenium was found to have a hexagonal close-packed, A3-type structure.[1-7] No other allotropic modifications were reported.

The melting point of 3453° ± 20°K reported by Sims, Craighead, and Jaffee[1] was adopted as the best value. Previous measurements had established values of 3440° ± 60°K[5] and 3433°K.[8]

b. Thermodynamic Properties

1) Heat of fusion

The heat of fusion of rhenium had not been measured. An entropy of fusion of 2.300 ± 0.440 e.u./gfw was assumed, corresponding to a heat of fusion of 7.942 kcal/gfw. An uncertainty of ± 1.500 kcal/gfw was assigned to the heat of fusion.

2) Entropy and heat content at 298.15°K

The low-temperature heat capacity of rhenium was measured by Keesom and Bryant,[9] Wolcott,[10] Horowitz and Daunt,[11] and Smith, Oliver, and Cobble.[12] Rhenium was found to have a superconducting transition at about 2°K.[13-15]

The adopted values for S°_{298} and $H^\circ_{298} - H^\circ_0$ were based on the measurements of Smith, Oliver, and Cobble[12] as was the value for S°_{298} tabulated by Kelley and King.[16] The C°_p value of 6.160 ± 0.04 cal/°K gfw at 298.15°K adopted herein represented a slight upward revision of the smoothed C°_p at that temperature given in the original reference. S°_{298} was calculated to be 8.886 ± 0.050 e.u./gfw, and $H^\circ_{298} - H^\circ_0$ was calculated to be 1.307 kcal/gfw.

3) High-temperature heat content

The high-temperature heat content of rhenium was measured by Jaeger and Rosenbohm.[8] Their data in cal/°K gfw were represented between 273° and 1474°K by the equation

$$C^\circ_p = 5.726 + 1.234 \times 10^{-3}\, T \quad . \qquad \text{(IVA4-1)}$$

Kelley[17] used a different equation on the basis of the same measurements

$$C_p^\circ = 5.660 + 1.300 \times 10^{-3}\,T \quad . \qquad \text{(IVA4-2)}$$

Sims and others[18] reported relative values of the heat capacity from 1620° to 2690°K obtained by a "hot-wire" method. These results had only limited precision. The data suggested, however, that the heat capacity was increasing with temperature more rapidly than a simple linear dependence. They adjusted the low-temperature portion of their data to the high-temperature portion of the results of Jaeger and Rosenbohm[8] and obtained thereby a heat capacity of about 9.5 cal/°K gfw at 2700°K. An extrapolation of Jaeger and Rosenbohm's data[8] would give a heat capacity of 9.06 cal/°K gfw at that temperature, and Kelley's equation[17] would give a value of 9.17 cal/°K gfw.

Jaeger and Rosenbohm's equation[8] gave a heat capacity approximately 0.06 cal/°K gfw lower than the adopted value at 298.15°K. To join the low-temperature data in cal/°K gfw to that of Jaeger and Rosenbohm[8] and also, follow the temperature dependence suggested by Sims and others[18] above 1600°K, the following equation was adopted for temperatures from 298°K to the melting point:

$$C_p^\circ = 5.883 + 0.876 \times 10^{-3}\,T + 0.0177 \times 10^{-5}\,T^2 \quad . \qquad \text{(IVA4-3)}$$

This equation agreed with the equation of Jaeger and Rosenbohm[8] to ± 0.02 cal/°K gfw between 500° and 1500°K.

In the absence of experimental data, the heat capacity of liquid rhenium was assumed to be 11.000 cal/°K gfw to be consistent with the above equations. An estimate of 10.8 cal/°K gfw was adopted by Stull and Sinke[19] from Sherwood and others.[20]

4) Standard heat of formation of the gas at 298.15°K and the boiling point

The vapor pressure of rhenium was measured by Sherwood and others.[20] The standard heat of formation of the gas at 298.15°K was herein calculated by the Third Law method to be 185.370 ± 1.500 kcal/gfw from their vapor-pressure data and the thermodynamic functions for rhenium tabulated herein. The normal boiling point and the corresponding heat of vaporization were calculated to be 5960.67 ± 260°K and 168.315 ± 12.940 kcal/gfw, respectively. These quantities did not differ greatly from those given by Stull and Sinke.[19]

5) Ideal gas properties

The ideal monatomic gas thermodynamic properties of rhenium previously reported[21] were retained.

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5. Rhodium

a. Crystal Structure and Melting Point

Elemental rhodium was found to have a face-centered cubic, A1-type structure at room temperature.[1, 2] An allotropic transformation at approximately 1000° C had been proposed from X-ray, heat-capacity, and thermoelectric measurements.[3-5] However, Bale[6] reported the electrical resistivity and lattice parameter to vary smoothly and continuously from room temperature to 1600° C with metal containing less than 10 ppm metallic impurities. He did observe anomalous behavior toward mechanical working and suggested that either rhodium was uniquely sensitive to impurities or had a mechanism for plastic behavior unlike other face-centered cubic metals. Strong and Bundy,[7] in the course of high pressure studies on "thermocouple-grade" rhodium, found the electrical resistivity to follow a fairly smooth curve up to the melting point but observed a volume contraction of the metal around 1000° to 1400° C. Rhodium was assumed in the present compilation to be face-centered cubic up to the melting point. However, this fact would need further verification.

The melting point of rhodium was taken to be 2239° ± 3°K from the measurements of Roeser and Wensel,[8] Barber and Schofield,[9] Oriani and Jones,[10] and Haworth and Hume-Rothery.[11]

b. Thermodynamic Properties

1) Heat of fusion

In the absence of an experimental determination of the heat of fusion of rhodium, an entropy of fusion of 2.300 e. u./gfw was assumed. The corresponding heat of fusion was 5.150 kcal/gfw to which an uncertainty of ± 0.800 kcal/gfw was assigned.

2) Entropy and heat content at 298.15°K

The low-temperature heat capacity of rhodium was measured by Budworth, Hoare, and Preston,[12] Wolcott,[13] and Clusius and Losa.[14] S°_{298} was taken to be 7.530 ± 0.050 e. u./gfw from Kelley and King's[15] evaluation of the data of Clusius and Losa.[14] $H^{\circ}_{298} - H^{\circ}_{0}$ was calculated to be 1.174 kcal/gfw from the same data. The heat-capacity value of 5.940 ± 0.070 cal/°K gfw at 298.15°K was obtained from an extrapolation of the low-temperature data.

3) High-temperature heat content

The high-temperature heat content of rhodium was measured by Holzmann,[16] and Jaeger and Rosenbohm.[5] These two sources gave equations leading to heat capacities which differed by about 0.20 cal/°K gfw at 298.15°K and by about 0.15 cal/°K gfw at 1200°K. The equations had somewhat different temperature dependences. According to Holzmann,[16] the equation in units of cal/°K gfw over the temperature range of 273° to 1173°K was

$$C_p^\circ = 5.707 + 1.883 \times 10^{-3}\,T \quad . \qquad \text{(IVA5-1)}$$

According to Jaeger and Rosenbohm,[5] the equation from 273° to 1573°K in the same units was

$$C_p^\circ = 6.015 - 0.869 \times 10^{-3}\,T + 4.343 \times 10^{-6}\,T^2 - 1.816 \times 10^{-9}\,T^3 \quad . \qquad \text{(IVA5-2)}$$

Both of these equations yielded heat capacities at 298.15°K larger than the adopted value. Jaeger and Rosenbohm's[5] data showed a maximum in the heat capacity, at about 1500°K, which they interpreted to be caused by an allotropic transition. They also gave results for the assumed high-temperature modification in the temperature range from 1665° to 1877°K.

The herein-adopted representation for the heat capacity of rhodium in cal/°K gfw from 298.15°K to the melting point is

$$C_p^\circ = 5.600 + 2.020 \times 10^{-3}\,T - \frac{0.2334 \times 10^5}{T^2} \quad . \qquad \text{(IVA5-3)}$$

This equation yields heat capacities which join smoothly with the low-temperature data and agree with the average of the results of Holzmann,[16] and Jaeger and Rosenbohm[5] between 500° and 1200°K. Above 400°K, it yields values that are 0.05 cal/°K gfw greater at a maximum than those from an equation selected by Kelley[17] to represent the same high-temperature data.

The heat capacity of liquid rhodium was assumed to be 10.000 cal/°K gfw.

4) Standard heat of formation of the gas at 298.15°K

The vapor pressure of rhodium was measured by Panish and Reif,[18] Hampson and Walker,[19] and Dreger and Margrave.[20]

A recalculation was made of ΔH°_{f298} with these vapor-pressure data by the Third Law method using the thermodynamic functions for rhodium tabulated herein. From the data of Panish and Reif,[18] the standard heat of formation at 298.15°K was calculated to be 132.900 ± 0.600 kcal/gfw. The data of Hampson and Walker[19] gave a value of 132.640 ± 1.500 kcal/gfw, and the data of Dreger and Margrave[20] gave a value of 134.400 ± 2.100 kcal/gfw. The value of 132.770 kcal/gfw was adopted as the best value from the first two sources, and an uncertainty of ± 1.600 kcal/gfw was assigned to it. The normal boiling point was calculated to be 3995.89° ± 130°K, and the heat of vaporization at the boiling point was found to be 118.145 ± 6.570 kcal/gfw. All of these quantities were very close to earlier estimates of Stull and Sinke.[21]

5) Ideal gas

The thermodynamic properties of the ideal monatomic gas previously reported[22] were retained.

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6. Technetium

a. Crystal Structure and Melting Point

Elemental technetium was found to have a hexagonal close-packed, A3-type structure.[1] No evidence for other crystalline modifications was found[2] at pressures up to 100,000 kg/cm^2 except for a superconducting phase below 11.2°K.[3] A melting point of 2413° ± 20°K was reported[4] from what was described as a "preliminary" measurement. More recently, the melting point was measured to be 2473° ±50°K.[5] The latter value was adopted herein.

b. Thermodynamic Properties

1) Heat of fusion

The entropy of fusion was assumed to be 2.300 e.u./gfw. This gave a heat of fusion of 5.688 kcal/gfw. An uncertainty of ±1.000 kcal/gfw was assigned to the heat of fusion.

2) Entropy and heat content at 298.15°K

S°_{298} for technetium was estimated to be 9.0 e.u./gfw in NBS Circular 500,[6] 8.0 e.u./gfw by Brewer,[7] and 7.4 e.u./gfw by Cobble.[8] For the present compilation, Brewer's[7] estimate was adopted with an uncertainty of ±0.500 e.u./gfw as recommended by Kelley and King.[9] The adopted value appeared to be the most consistent with S°_{298} values for neighboring elements in the periodic table. $H^\circ_{298} - H^\circ_0$ was estimated to be 1.230 kcal/gfw.

3) High-temperature heat capacity

Experimental measurements were not available. Kelley[10] gave an equation for the high-temperature heat capacity of technetium in cal/°K gfw based on heat-content estimates by Brewer;[7] i.e.,

$$C^\circ_p = 5.200 + 2.000 \times 10^{-3}\,T \quad . \qquad \text{(IVA6-1)}$$

This equation was adopted herein.

The heat capacity of liquid technetium was estimated to be 10.000 cal/°K gfw.

4) Standard heat of formation of the gas at 298.15°K

The estimate for ΔH°_{f298} of 155.000 kcal/gfw by Stull and Sinke[11] was adopted herein and assigned an uncertainty of ±5.000 kcal/gfw. This estimate was based on vapor-pressure estimates of Brewer.[7]

The normal boiling point and the corresponding heat of vaporization were calculated to be 4840.07° ±500°K and 139.871 ±13.2 kcal/gfw, respectively.

5) Ideal gas

The thermodynamic functions of the ideal monatomic gas of Tc reported earlier[12] were retained.

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7. Thorium

a. Crystal Structure, Transition Point, and Melting Point

Elemental thorium was found to have a face-centered cubic, A1-type structure from room temperature to 1360°C and a body-centered cubic A2 structure[1-3] from 1360°C to the melting point. The transition point and, in particular, the melting point had been found to be very sensitive to the kind and amount of impurities. Summaries of the earlier and frequently discordant results were found in numerous review publications on thorium.[4-7] Kelley,[8] and Stull and Sinke[9] adopted an α–β transition temperature of 1400°C[1] and a melting point of 1695°C[10] from earlier measurements of Chiotti. In 1955, Chiotti[4] recommended a melting point of 1750°C. Later, he quoted unpublished studies of Chiotti and Tentor[11] as leading to a value of 1360°C for the transition point and of 1755°C for the melting point. The latter temperatures were adopted for the present compilation. The transition temperature had also been determined to be 1363° ± 10°C by McMasters and Larsen[12] and to be 1330° ± 20°C by Wilson, Austin, and Schwartz.[3] Bentle[13] reported a plot of phase data which seemed to place the α–β transition around 1350° to 1360°C.

b. Thermodynamic Properties

1) Heat of transition and fusion

The heats of transition and fusion of thorium had not been measured. Although no thermal arrest was noted by some observers on cooling massive amounts of liquid thorium, such an arrest had been observed by Miller[4] at 1626°C. The rapid solidification of liquid thorium on casting had been cited as evidence for an unusually low heat of fusion.[4] However, phase data for some thorium systems had been analyzed[4] to indicate a heat of fusion of the order of 4 kcal/gfw. For the present compilation, the estimates of Stull and Sinke[9] of 0.4 e.u./gfw for the entropy of transition and 1.9 e.u./gfw for the entropy of fusion were adopted. The corresponding heats of transition and fusion were 0.653 ± 0.200 kcal/gfw and 3.853 ± 1.000 kcal/gfw, respectively.

2) Entropy and heat content at 298.15°K

The low-temperature heat capacity of thorium was measured by Smith and Wolcott[14] and by Griffel and Skochdopole.[15] Griffel and Skochdopole calculated S°_{298} to be 12.760 e.u./gfw and $H^{\circ}_{298} - H^{\circ}_{0}$ to be 1.556 kcal/gfw from their data. Kelley and King[16] gave an uncertainty of ± 0.2 e.u./gfw to the entropy value. This relatively large uncertainty was due primarily to an uncertainty in the entropy below 20°K, which was in turn due to differing values of the electronic heat capacity from the data of Smith and Wolcott,[14] and Griffel and Skochdopole.[15] Clusius and Franzosini[17] attributed the differing electronic heat capacities to differing sample purity.

Thorium has been found to be a superconductor below 1.4°K.[18,19]

3) High-temperature heat content

The high-temperature heat content of thorium was measured by Jaeger and Veenstra,[20] and the high-temperature heat capacity was measured by Wallace,[21] and Mitkina.[22] The measurements of Jaeger and Veenstra[20] were made on metal containing 6.04 percent ThO_2. A correction to the observed heat content was therefore necessary. The tabulations of Kelley,[8] and Stull and Sinke [9] were based on these corrected data. The tabulated data did not reproduce the corrected data of Jaeger and Veenstra[20] particularly well, probably because the last were modified further to give the heat capacity at 298.15°K from the low-temperature data of Griffel and Skochdopole.[15] However, neither the corrected data nor their modification by Kelley[8] joined smoothly with the low-temperature results. The corrected data gave a heat capacity at 298.15°K that was much too large, and their modification gave a temperature coefficient of the heat capacity near room temperature at variance with the low-temperature measurements.

The high-temperature heat-capacity data of Wallace[21] were obtained by a pulse-heating method on 10-mil thorium wires. These data joined smoothly with the low-temperature data. Above a temperature of approximately 500°K, a contribution to the heat capacity in addition to the contributions of lattice vibrations $C_p - C_v$ and the electronic heat capacity was observed which fitted a Schottky-type equation. This excess was attributed by Wallace[21] to thermal excitation of electrons to a narrow energy band above or below the Fermi level, and not to defect formation. A similar interpretation was made[23] of the heat-capacity measurements on uranium.[24] The results of Wallace[21] were adopted for this compilation and extrapolated to the α–β transition at 1633°K. These data in cal/°K gfw were represented by the following pair of equations over the temperature ranges of 298° to 800°K and 800° to 1633°K, respectively:

$$C_p^{\circ} = 5.773 + 2.548 \times 10^{-3}\,T \quad , \tag{IVA7-1}$$

$$C_p^{\circ} = 5.553 + 4.928 \times 10^{-3}\,T - 4.703 \times 10^{-6}\,T^2 + 2.590 \times 10^{-9}\,T^3 \quad . \tag{IVA7-2}$$

The technique used by Mitkina[22] gave a heat capacity that was too low at room temperature and increased too rapidly with temperature to 700°K.

The estimate of 11.000 cal/°K gfw for the heat capacities of both β-Th and liquid thorium made by Kelley,[8] and Stull and Sinke [9] was adopted herein.

4) Standard heat of formation of the gas at 298.15°K

Thorium vapor-pressure data had been reported by Zwikker,[25] Andrews,[26] deBoer,[27] Darnell, McCollum, and Milne,[28] and Goldwater and Danforth.[29]

Most tabulations of thorium vapor pressures were taken from Brewer,[30] who combined the data of Zwikker,[25] and deBoer.[27] Dushman[31] and Lofthus[32] also gave compilations based on Zwikker's[25] results. The original vapor-pressure data were not given by Zwikker,[25] and deBoer,[27] so that it was possible to calculate only a rough value of the standard heat of formation of the gas with the thermodynamic functions given herein. If the various representations of these early data were all used, the heat of sublimation at 298.15°K would vary from 130 to 140 kcal/gfw.

The data of Andrews[26] gave a heat of formation that was much too high, probably due to the evaporation of ThO_2 rather than thorium.

For the present compilation, the vapor-pressure data of Darnell, McCollum, and Milne[28] were adopted. A standard heat of formation of the gas at 298.15°K of 137.700 ± 1.000 kcal/gfw was derived by the Third Law method. The last authors discussed the high evaporation rates from thorium containing ThO_2 due to the formation of ThO(g) from the reaction of thorium with ThO_2.

The smoothed evaporation-rate data of Goldwater and Danforth[29] gave a heat of formation that was 10 or more kcal/gfw too low and quite temperature-dependent.

The normal boiling point and associated heat of vaporization were calculated to be 5060.26° ± 440°K and 122.765 ± 15.060 kcal/gfw, respectively. This boiling point was 560°K higher than the previous estimate of Brewer.[30]

5) Thermodynamic functions of ideal monatomic gas

The thermodynamic functions of ideal monatomic thorium gas were calculated from the energy levels given by Zalubas.[33] The functions so calculated must be regarded as tentative since the analysis of the thorium spectrum was incomplete.[33]

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B. COMPOUNDS

1. Calcium Oxide (CaO)

a. Condensed Phases

Values of ΔH_f°, ΔF_f°, and $\log_{10}K_p$ were calculated using $\Delta H_{f298}^\circ = -151.410$ kcal/gfw* for CaO(s) from the combustion results of Huber and Holley;[1] their paper contained a discussion of earlier determinations. An uncertainty of ±0.500 kcal/gfw was assigned to this value of ΔH_{f298}°.

Previously reported[2] thermodynamic functions on CaO condensed phases were retained.

b. Gaseous Calcium Oxide

Thermodynamic functions for CaO(g) had been calculated on the basis of a $^1\Sigma$ ground state and were reported in the first summary technical report.[2] They were recalculated with the assumption that the ground state is $^3\Sigma$.

As is also the case for MgO(g) and SrO(g), dissociation energies determined from the known singlet system of CaO(g) are significantly lower than dissociation energies calculated from thermochemical data. In assuming that the discrepancy may be resolved by adopting a ground state as yet unobserved, the implicit assumptions have also been made that the Birge-Sponer extrapolation from the lowest singlet state to the lowest possible states of Ca and O is correct, and that polymeric molecules such as Ca_2O_2 are not important.

Although the assumption of a triplet ground state is reasonable, the assumption that it is $^3\Sigma$ is on less firm ground since it may be $^3\pi$ or $^3\Delta$. However, for the present compilation, a $^3\Sigma$ ground state has been assumed for MgO(g), CaO(g), and SrO(g). It has also been assumed that the lowest $^1\Sigma$ state is 15000 cm^{-1} above the $^3\Sigma$ ground state. This interval has been derived by decreasing the analogous interval of 19200 cm^{-1} adopted for MgO(g). A second $^3\Sigma$ state at 20000 cm^{-1} has also been assumed.

Spectroscopic constants for the triplet states were estimated. The spectroscopic constants used in the calculation were (in units of cm^{-1}) as follows:

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*The value, −151.900 kcal/gfw, given by Huber and Holley[1] was apparently based on an atomic weight of 40.18 for Ca.

State	E	ω_e	$\omega_e x_e$	B_e	α_e	D_e(x 10^6)
X $^3\Sigma$	(0	850.0	5.0	0.53	0.004	0.7)
X′ $^1\Sigma$	(15000)	732.11	4.81	0.44447	0.00335	0.656
$^3\Sigma$	(20000	725.0	4.0	0.45	0.003	0.7)
A $^1\Sigma$	26600	716.0	1.60	0.4063	0.00141	0.54
B $^1\pi$	40900	580.0	2.80	0.3882	0.0055	0.7
C $^1\Sigma$	43800	560.9	4.0	0.3731	0.0032	0.7

Spectroscopic constants between parentheses were estimated. Constants for the singlet states were those used previously,[2] with the exception of an addition of 15000 cm^{-1} to E.

A copious literature existed in which thermochemical data had been used to derive the dissociation energy of CaO(g). None of the work could be regarded as definitive; however, most of it could be interpreted as showing that CaO vaporized primarily by dissociation to the gaseous elements. Past work had been reviewed by the following authors who selected the indicated dissociation energies at 0°K:

Source	D°_0
	kcal/gfw
Brewer[3]	103 ± 8
Brewer[4]	90 ± 12
Gaydon[5]	108 ± 12
Ackermann, Thorn, and Winslow[6]	99

A dissociation energy of 100 kcal/gfw was adopted herein. With this dissociation energy and appropriate thermodynamic functions for CaO(g), O, and Ca from the present compilation, ΔH°_{f298} for CaO(g) was calculated to be 0.800 kcal/gfw. An uncertainty of ±15 kcal/gfw was assigned to it.

A vaporization temperature, the temperature at which the sum of the partial pressures of all vaporizing species (excepting any polymeric species) equaled 1 atm, was calculated assuming the existence of equilibrium between O and O_2. The temperature so calculated was 3890°K. The partial pressure of undissociated CaO(g) at that temperature was 0.31 atm. An observed boiling point of 3900°K was reported by Mott.[7]

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6. Ackermann, R.J., R.J. Thorn, and G.H. Winslow, Planet. Space Sci. 3, 12 (1961).

7. Mott, W.R., Trans. Am. Electrochem. Soc. 34, 255 (1918).

2. Cerium Monoxide (CeO)

Vibrational constants used in the calculation of the thermodynamic functions of CeO(g) were taken from Herzberg.[1] In the absence of a rotational analysis, a value of B_e for the ground state was calculated from an estimated internuclear distance of 1.81Å. Values of B_e for higher electronic states were estimated from the assumption that the ratio ω_e/B_e was constant for all electronic states. D_e's were estimated from the relation $D_e = 4B_e^3/\omega_e^2$.

Herzberg[1] listed two systems of states for CeO(g) between which the intercombination energy was unknown. None of the states had been classified. It was assumed that each of the states listed by Herzberg had a multiplicity of 2, and that the state designated by him as (X′) was 13700 cm^{-1} above the state designated as (X).

Spectroscopic constants used for the calculation of thermodynamic functions of CeO(g) were (in units of cm^{-1} where applicable) as follows:

State	E	ω_e	$\omega_e x_e$	B_e	D_e (x 10^7)	g
(X)	0	865.0	2.99	(0.359)	(2.5)	(2)
A	12764.3	785.3	2.13	(0.326)	(2.2)	(2)
B	13817.2	788.3	1.76	(0.327)	(2.3)	(2)
(X′)	(13720.0)	840.2	2.58	(0.349)	(2.3)	(2)
D	(34276.0)	791.7	1.72	(0.329)	(2.3)	(2)
E	(34584.0)	807.9	2.04	(0.335)	(2.3)	(2)

Quantities in parentheses were estimated in whole or in part.

Walsh, Dever, and White[2] made a mass spectrometric study of the reaction

$$Ce(g) + LaO(g) \rightleftharpoons La(g) + CeO(g) \quad . \qquad (IVB2-1)$$

From this study of the reaction, it was reported that

$$\Delta H^\circ_{1870} = 1.05 \pm 0.20 \text{ kcal/gfw} \quad , \qquad (IVB2-2)$$

and

$$\Delta S^\circ_{1870} = 0.33 \pm 0.12 \text{ cal/}^\circ\text{K gfw} \quad . \qquad (IVB2-3)$$

Therefore, the difference between dissociation energies was

$$D^{\circ}_{1870}\,(\mathrm{LaO}\,(g)) - D^{\circ}_{1870}\,(\mathrm{CeO}\,(g)) = 1.05 \pm 0.20\ \mathrm{kcal/gfw} \quad . \qquad (\mathrm{IVB2\text{-}4})$$

With the acceptance of the assumption of the latter authors that $\Delta H^{\circ}_{187} = \Delta H^{\circ}_{0}$, then there resulted the relations

$$D^{\circ}_{0}\,(\mathrm{CeO}\,(g)) = D^{\circ}_{0}\,(\mathrm{LaO}\,(g)) - (1.05 \pm 0.20) \qquad (\mathrm{IVB2\text{-}5})$$

$$= (186.3 \pm 4.7) - (1.05 \pm 0.20) \qquad (\mathrm{IVB2\text{-}5a})$$

$$= 185 \pm 5\ \mathrm{kcal/gfw} \quad . \qquad (\mathrm{IVB2\text{-}5b})$$

D°_{0} for LaO(g) was that given by Goldstein, Walsh, and White.[3] The value of ΔH°_{f298} for CeO(g) calculated from this D°_{0} was -31.100 kcal/gfw; an uncertainty of ± 5.000 kcal/gfw was assigned to it.

REFERENCES FOR SECTION IVB2

1. Herzberg, G., Molecular Spectra and Molecular Structure, I. Spectra of Diatomic Molecules, 2nd ed., Van Nostrand, New York (1950).

2. Walsh, P. N., D. F. Dever, and D. White, J. Phys. Chem. 65, 1410 (1961).

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3. Magnesium Oxide (MgO)

a. Condensed Phases

The melting point of magnesium oxide was measured and reported by McNally, Peters, and Ribbe[1] to be 3098° ± 20°K.

The value of ΔH°_{f298} for solid MgO reported by Holley and Huber,[2] -143.7 kcal/gfw, was adopted herein. This value, obtained by combustion calorimetry, was in excellent agreement with the value of -143.84 kcal/gfw determined by Shomate and Huffman[3] from the heat of solution of MgO in HCl. Moose and Paar[4] had earlier reported the value -146.1 kcal/gfw for this heat of formation. No weight was given to this last value in assigning an uncertainty of ± 0.5 kcal/gfw.

The table of thermodynamic functions for the condensed phases of MgO was revised to incorporate the new melting point, maintaining the heat of fusion as 18.5 kcal/gfw. Other properties previously reported[5] were retained.

b. Gaseous Magnesium Oxide

As previously noted,[5] it was not certain that the lowest state of the singlet systems of MgO(g) was the ground state of the molecule. As a matter of fact, the best evidence was to the contrary. The previous table of the thermodynamic functions of MgO(g),[5] which adopted a $^1\Sigma$ ground state was replaced by the result of a new calculation based on a $^3\Sigma$ ground state.

Brewer and Porter[6] observed several ultraviolet systems for MgO(g) which they interpreted as evidence for adjacent $^3\Sigma$ and $^3\pi$ states lying 55 ± 15 kcal/gfw below the lowest $^1\Sigma$ state. It had been shown[7-9] that parts of their systems were probably due to MgOH and polymers containing Mg and O. Thrush[10] had recently reported, however, that only Brewer and Porter's system-I was observed in absorption, and that this spectrum was unaffected by the addition of water.

In the revised calculations of the thermodynamic functions of MgO(g) reported herein, Brewer and Porter's[6] vibration analysis of their system-I (taken to be due to transitions between $^3\Sigma$ states) was adopted. The low-lying $^1\Sigma$ state was taken to be 55 kcal/gfw (19,200 cm^{-1}) above the $^3\Sigma$ ground state. Bulewicz and Sugden[9] reported this interval to be 45 kcal/gfw. Values of B_e for the triplet states were estimated from an average B_e/ω_e ratio of analyzed singlet states. The spectroscopic constants used for the revised calculation of the thermodynamic functions were (in units of cm^{-1}) as follows:

State	E	ω_e	$\omega_e x_e$	B_e	α_e	$D_e (x\,10^6)$
X $^3\Sigma$	0	902	13.0	0.625	0.0094	1.2
$^3\Sigma$	26863.9	817	9.5	0.585	0.008	1.2
X′ $^1\Sigma$	19200.	782.84	5.15	0.5711	0.005	1.22
A $^1\pi$	22694.4	664.4	3.91	0.5056	0.0046	1.2
B $^1\Sigma$	39204.7	824.1	4.76	0.5822	0.0045	1.2

Dissociation energy values at 0°K for MgO(g) ranging from 85 to 120 kcal/gfw had been reported. The spread of values was due in part to different assumptions as to the ground state of the molecule and, in part, to experimental difficulties in determining relative amounts of dissociated and undissociated vaporizing species. A Birge-Sponer extrapolation of the singlet system gave 85 kcal/gfw for D_0^o. Porter, Chupka, and Inghram[11] reported D_0^o to be less than < 90 kcal/gfw ($^3\Sigma$ ground state) from mass spectrometric studies in which vaporization was due to the gaseous elements at 1950°K. However, it was possible that the experimental arrangement actually provided reducing conditions.[12]

From flame studies, Huldt and Lagerqvist[13] reported D_0^o to be 120 kcal/gfw ($^1\Sigma$ ground state), a value which was recalculated to 115 kcal/gfw ($^3\Sigma$ ground state) by Brewer and Porter.[6] From vapor-pressure measurements, Brewer and Porter[6] reported a heat of sublimation at 298.15°K of 130 kcal/gfw, which corresponded to a D_0^o of 108 kcal/gfw ($^3\Sigma$ ground state). Flame photometry studies of Bulewicz and Sugden gave 98 ± 2 kcal/gfw ($^3\Sigma$ ground state) for D_0^o. Veits and Gurvich,[14, 15] using a flame technique, reported D_0^o to be 100 kcal/gfw. Gaydon[16] recommended a value of 104 ± 16 kcal/gfw for this quantity.

For the present compilation, D_0^o was taken to be 105 kcal/gfw, which corresponded to a ΔH_{f298}^o for MgO(g) of -11.1 kcal/gfw. An uncertainty of ± 15 kcal/gfw was assigned to ΔH_{f298}^o.

The vaporization temperature of MgO, the temperature at which the sum of the partial pressures of all vaporizing species equals 1 atm has been calculated. The assumption has been made that vaporization by dissociation produces equilibrium amounts of O and O_2. The vaporization temperature so calculated is 3110°K, which is very near the melting point. It has been calculated that the principal vaporizing species is undissociated MgO(g). Required data have not been available for an estimate of contributions of possible polymeric species. Mott[16] has reported the boiling point of MgO to be 3900°K.

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4. Moose, J. E. and S. W. Paar, J. Am. Chem. Soc. 46, 2656 (1924).
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16. Mott, W. R., Trans. Am. Electrochem. Soc. 34, 255 (1918).

4. Manganese Oxide (MnO)

The spectroscopic constants used for the calculation of the thermodynamic functions of MnO(g) were (in units of cm^{-1}) as follows:

E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	D_e (x 10^7)
0	839.55	4.79	---	0.499	7.1
17909.59	762.75	9.60	0.06	0.453	6.4

The vibrational constants for the two electronic states were from Das Sarma,[1] who modified the constants reported by Herzberg[2] for the same two states. Das Sarma calculated a dissociation energy at 0 °K of 95 kcal/gfw for the lower state by a Birge-Sponer linear extrapolation of his data. From volatility studies on MnO, Brewer and Mastick[3] concluded that D_0° was less than 106 kcal/gfw. From flame studies, Huldt and Lagerqvist[4] reported D_0° to be 92 ± 9 kcal/gfw. Because of the agreement between the thermochemical and spectroscopic values of D_0°, the lower of the two electronic states was taken to be the ground state of MnO(g).

A rotational analysis of the states had not been made. The internuclear distance of the ground state was estimated to be 1.65Å corresponding to a value of 0.499 cm^{-1} for B_e. The internuclear distance for the ground state was estimated to be 1.67Å by Brewer and Chandrasekharaiah[5] and 1.79Å by Das Sarma.[1] B_e for the upper electronic state was estimated to be 0.453 cm^{-1} from the assumption that ω_e/B_e would be a constant ratio for the various electronic states of a given molecule. Values of D_e were estimated from the relation $D_e = 4\,B_e^3/\omega_e^2$. The statistical weights of the ground and excited electronic states were assumed to be 4 and 2, respectively.

D_0° for MnO(g) was taken to be 95 kcal/gfw from Das Sarma.[1] With appropriate thermodynamic functions from the present compilation, ΔH°_{f298} was calculated to be 30.600 kcal/gfw. An uncertainty of ± 10.000 kcal/gfw was assigned to this quantity.

REFERENCES FOR SECTION IVB4

1. Das Sarma, J. M., Z. Physik. 157, 98 (1959).

2. Herzberg, G., Molecular Spectra and Molecular Structure, I. Spectra of Diatomic Molecules, 2nd ed., Van Nostrand, New York (1950).

3. Brewer, L. and D. F. Mastick, J. Chem. Phys. 19, 834 (1951).

4. Huldt, L. and A. Lagerqvist, Arkiv Fysik 3, 525 (1952).

5. Brewer, L. and M. S. Chandrasekharaiah, U. S. At. Energy Comm. Rept. UCRL-8713 (Rev.) (1960).

5. Platinum Monoxide (PtO)

No spectroscopic data were available for PtO(g). The calculation of the thermodynamic functions was made with the assumption that the molecule was a harmonic oscillator. The vibration frequency was estimated to be 785 cm^{-1}. From an estimated internuclear distance of 1.85Å, a value for B_e of 0.334 cm^{-1} was calculated. A multiplicity of 6 was assumed for the single electronic state used in the calculation.

The dissociation energy of PtO(g) at 0°K was taken to be one-half that for PtO_2[1,2] or 105 kcal/gfw. The value of ΔH°_{f298} calculated from this value of D°_{0} was 88.6 kcal/gfw. An uncertainty of ± 15 kcal/gfw was assigned to ΔH_{f298} .

REFERENCES FOR SECTION IVB5

1. Brewer, L. and M. Rosenblatt, Chem. Rev. 61, 257 (1961).

2. Alcock, C. B., Plat. Met. Rev. 5, 134 (1961).

6. Rhenium Oxide (ReO)

No spectroscopic data were available for gaseous ReO. The following values of ω_e and r_e were estimated for this molecule:

ω_e	r_e	B_e
cm^{-1}	Å	cm^{-1}
858 (760)	1.80 (1.82)	0.355

Values in parentheses were estimated by Brewer and Chandrasekharaiah.[1] B_e was calculated from the estimated r_e by the relation

$$B_e = \frac{1.686 \times 10^{-15}}{\mu r_e^2} , \qquad \text{(IVB6-1)}$$

where B_e is in units of cm^{-1}, μ is the reduced mass in mass units, and r_e, the equilibrium internuclear distance, is in cm.

Thermodynamic functions for gaseous ReO were calculated with the above constants (equivalent to assuming that the molecule is a rigid rotator and harmonic oscillator) from the assumption of the existence of only a ground electronic state with a statistical weight of 4.

D_0^o for ReO(g) was estimated to be 154 kcal/gfw from a comparison of adopted dissociation energies of monoxides of elements neighboring rhenium in the periodic table. A ΔH_{f298}^o for ReO(g) of 90.000 kcal/gfw was then calculated with appropriate thermodynamic functions from the present compilation. An uncertainty of ±15.000 kcal/gfw was assigned to ΔH_{f298}^o .

REFERENCE FOR SECTION IVB6

1. Brewer, L. and M. S. Chandrasekharaiah, U. S. At. Energy Comm. Rept. UCRL-8713 (Rev.) (1960).

7. Rhodium Monoxide (RhO)

In the absence of spectroscopic data, the RhO(g) molecule was assumed to be a rigid rotator and harmonic oscillator. The vibration frequency was estimated to be 820 cm^{-1}. B_e was taken to be 0.373 cm^{-1} from an estimated internuclear distance of 1.81Å. A multiplicity of 4 was assumed for the single electronic state used in the calculation.

The dissociation energy of RhO(g) at 0°K was assumed to be one-half that of the corresponding quantity for $RhO_2(g)$,[1,2] or 103 kcal/gfw. From the assumed D_0^o, ΔH^o_{f298} was calculated to be 88.4 kcal/gfw. An uncertainty of ± 15 kcal/gfw was assigned to ΔH^o_{f298}.

REFERENCES FOR SECTION IVB7

1. Brewer, L. and M. Rosenblatt, Chem. Rev. 61, 257 (1961).
2. Alcock, C. B., Plat. Met. Rev. 5, 134 (1961).

8. Strontium Oxide (SrO)

a. Condensed Phases

For the calculation of the ΔH_f°, ΔF_f°, and $\log_{10} K_p$ of the condensed phases of SrO, ΔH_{f298}° was taken to be -141.100 kcal/gfw from NBS Circular 500.[1] An uncertainty of ± 2.000 kcal/gfw was assigned to ΔH_{f298}°. Other data previously used for a hand calculation[2] were retained, and the thermodynamic functions were recomputed by machine.

b. Gaseous Strontium Oxide

The thermodynamic functions for SrO(g) were recalculated with an assumed $^3\Sigma$ ground state. (The reasons for this are discussed in the sections on MgO and CaO.) For SrO(g), the multiplicity of the lowest observed $^1\Sigma$ state was increased to 3; however, that of the other singlet states was unchanged. This was equivalent to placing the start of the singlet system approximately 10,000 cm^{-1} above the assumed triplet ground state. No other triplet states of greater electronic energy were assumed to exist. Spectroscopic constants used in the calculation were given previously.[2]

As also noted in the cases of MgO(g) and CaO(g), a discrepancy existed between the thermochemical and spectroscopic values of the dissociation energy of SrO(g). In all these cases, it had been generally assumed that the spectroscopic values were too low because the lowest lying singlet states to which they referred were not the ground states. However, because of experimental difficulties, even the thermochemical experiments did not give unambiguous results for SrO(g). The thermochemical dissociation energy values at 0°K, as derived from the various thermochemical experiments, had been reviewed by the following authors who preferred the indicated values:

Source	D_0°
	kcal/gfw
Brewer[3]	111 ± 4
Brewer[4]	83 ± 5
Gaydon[5]	106 ± 12
Ackermann, Thorn, and Winslow[6]	111

For the present compilation, a dissociation energy at 0°K of 110 kcal/gfw was selected. This value was derived from a partial pressure of SrO(g) of 1.06×10^{-10} atm at 1500°K and appropriate thermodynamic functions for SrO, O, and Sr from the present compilation. The indicated partial pressure of SrO(g) at 1500°K was calculated by Ackermann and Thorn[7] from the vapor-pressure measurements of Moore, Allison, and Struthers.[8] From flame studies, Lagerqvist and Huldt[9] determined D_0° to be 106 kcal/gfw, and Veits and Gurvich[10] reported the value to be 111 kcal/gfw.

A value for the ΔH_{f298}° of SrO(g) equal to -12.300 kcal/gfw was calculated from the adopted D_0° and appropriate thermodynamic functions for SrO(g), Sr, and O from the present compilation. An uncertainty of ± 10 kcal/gfw was assigned to ΔH_{f298}° .

The sum of the partial pressures of all vaporizing species was calculated to equal 1 atm at 4500°K. Vaporization was found by calculation to proceed principally to undissociated SrO(g); and at the vaporization temperature, the partial pressure of SrO(g) was calculated to be 0.78 atm.

REFERENCES FOR SECTION IVB8

1. Rossini, F. et al, Selected Values of Chemical Thermodynamic Properties, Natl. Bur. Standards (U.S.), Circ. 500 (1952).

2. Barriault, R. J. et al, Thermodynamics of Certain Refractory Compounds, Pt. I, Vol. 1, ASD TR 61-260 (31 October 1961).

3. Brewer, L., Chem. Rev. 52, 1 (1953).

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9. Technetium Oxide (TcO)

No spectroscopic data were available for gaseous TcO. The following values of ω_e and r_e were estimated for this molecule.

ω_e	r_e	B_e
cm^{-1}	Å	cm^{-1}
854	1.78 (1.77)	0.385

Values in parentheses were estimated by Brewer and Chandrasekharaiah.[1] B_e was calculated from the estimated r_e by the relation

$$B_e = \frac{1.686 \times 10^{-15}}{\mu r_e^2} , \qquad \text{(IVB9-1)}$$

where B_e is in units of cm^{-1}, μ is the reduced mass in mass units, and r_e, the equilibrium internuclear distance, is in cm.

Thermodynamic functions for gaseous TcO have been calculated with the above constants; this is equivalent to assuming that the molecule is a rigid rotator and harmonic oscillator, and that there exists only a ground electronic state with a statistical weight of 4.

D_0^o for TcO(g) was estimated to be 125 kcal/gfw from a comparison of adopted dissociation energies of monoxides of elements neighboring technetium in the periodic table. A ΔH_{f298}^o for TcO(g) of 88.600 kcal/gfw was then calculated with appropriate thermodynamic functions from the present compilation. An uncertainty of ± 15.000 kcal/gfw was assigned to ΔH_{f298}^o.

REFERENCE FOR SECTION IVB9

1. Brewer, L. and M. S. Chandrasekharaiah, U. S. At. Energy Comm. Rept. UCRL-8713 (Rev.) (1960).

10. Thorium Monoxide (ThO)

Calculations of the thermodynamic functions of gaseous thorium monoxide were based on the fragmentary spectroscopic data of Krishnamurty[1] and an estimated vibration frequency and internuclear distance. Krishnamurty reported lower electronic energy levels of 0, 2721, and 4177 cm^{-1}, which he suggested were due to the splitting of a $^3\pi$ ground state. This suggestion was adopted herein. The vibration frequency was estimated to be 800 cm^{-1}, and the Th-O bond distance was taken to be 1.86Å. No attempt was made to estimate the contribution of higher electronic energy levels. Spectroscopic constants derived from the above assumptions and used in the calculation of thermodynamic functions were (in units of cm^{-1})as follows:

State	E	ω_e	$\omega_e x_e$	B_e	α_e	$D_e (x 10^7)$
$X\ ^3\pi$	0 2721 4177	800	3.5	0.327	0.0018	2.2

The vibration frequency had been estimated by Krishnamurty[1] to be 740 cm^{-1}. The internuclear distance was estimated by Darnell, McCollum, and Milne[2] to be 1.93 ± 0.04Å from that frequency and Badger's rule. By using these last two quantities and Brewer and Chandrasekharaiah's[3] method of estimating the electronic partition function from the energy states of the + 2 ion, Darnell, McCollum, and Milne[2] calculated the entropy of ThO(g) at 1883°K to be 79.3 e.u./gfw. This entropy was about 3.8 e.u./gfw higher than the entropy at this temperature calculated herein.

In the course of studies on the vapor pressure of thorium metal, Darnell, McCollum, and Milne[2] made vaporization-rate measurements on the metal containing ThO_2. The high rates of vaporization in such a system was explained by the formation of ThO(g) via the reaction

$$Th(s) + ThO_2(s) \longrightarrow 2\,ThO(g) \qquad \text{(IVB10-1)}$$

From their assumption that the vaporization rates observed were for a system in equilibrium and that the activities of $ThO_2(s)$ and Th(s) were unity, the standard heat of formation of ThO(g) at 298.15°K was recalculated with the thermodynamic functions for the metal and ThO(g) given herein, thermodynamic functions for $ThO_2(s)$ from Kelley,[4] and the heat of formation of $ThO_2(s)$ from Huber, Holley, and Meierkord.[5] The value obtained for ΔH^{o}_{f298} was -7.640 kcal/gfw. This heat of formation would correspond to a dissociation energy at 0°K of 204 kcal/gfw. The dissociation energy of ThO(g) had been estimated by Brewer[6] to be 200 ± 20 kcal/gfw.

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V. EXPERIMENTAL STUDIES ON BORON OXIDE AND HYDROXIDE VAPORS

A. BORON

Boron exists in the earth's crust to the extent of only 1 part in 10,000 by weight. Nevertheless, it is one of the most important elements. In addition to its essential role in the growth of basic foodstuffs, it has many important applications in modern technology. Of particular interest in flight technology is the use of boron as a high-energy fuel and the use of its compounds as refractory insulation materials.

The many special physical and chemical properties of boron and its compounds are, of course, a consequence of the structure of the boron atom. Primarily, it is the small size of the atom which determines its unique properties as exemplified by the filling in of the crystal lattices of the heavier metals with interstitial boron to form hard, refractory metal borides.

The properties of boron and their relationship to the atomic structure are discussed in treatises on inorganic chemistry, and they do not need to be reviewed in detail here, except perhaps to mention the peculiar chemical valency of boron. Since there are only five electrons; i.e., two 1s, two 2s, and one 2p; boron experiences certain difficulties in forming the chemist's "stable octet," and many of its compounds are described as "electron-deficient." Much effort has been expended by chemists and physicists in acquiring an understanding of the molecular structure of these compounds. Research on almost all aspects of the physical and chemical properties of boron and its compounds is presently being actively pursued.

B. BORON OXIDES AND HYDROXIDES

The present study is concerned with oxygenated compounds of boron which exist in the vapor state in equilibrium with condensed phases. The known boron oxide vapors are BO, BO_2, B_2O_2, and B_2O_3. The only hydroxide vapor identified in appreciable amounts is metaboric acid, O=B-OH. Salts of metaboric acid can also exist as vapors. Orthoboric acid, $B(OH)_3$, and its salts are known primarily in the condensed phase or in solution; only trace amounts of $B(OH)_3$ vapor have been detected in equilibrium with H_2O and HBO_2 at high temperatures. Organic derivatives of orthoboric acid, such as tri-alkyl borates, are stable compounds which are easily vaporized at low temperatures; of course, they belong to a realm of chemistry completely different from the one under study.

Because of the many experimental difficulties associated with the study of highly refractory vapors, the investigation of boron-containing vapors has not progressed rapidly until recent years. Two methods of investigation have been especially useful when applied to these vapors; i.e., (1) the effusion-cell method with mass spectroscopic identification, and (2) optical spectroscopy; the latter method is used in the present study. These two methods obtain complementary data; e.g., the effusion cells and mass spectrometers give vapor pressures and species identification, while the optical spectrometers give information on the molecular structures and vibration frequencies. It is therefore appropriate to review some of the effusion-cell work before discussing the optical spectroscopic studies in detail.

1. Effusion-Cell Studies

Inghram, Porter, and Chupka[1] analyzed the vapor effusing from a Knudsen cell containing a mixture of boron and B_2O_3 and found it to be mainly B_2O_2. For the heat-of-vaporization B_2O_2 (g), they calculated $\Delta H_{1400°K} = 94 \pm 8$ kcal/mole. For the reaction $2/3\ B(s) + 2/3\ B_2O_3\ (g) \rightarrow B_2O_2\ (g)$, they obtained $\Delta H_0^o = 35.7 \pm 3.5$ kcal/mole. They estimated the heat-of-dimerization $2BO \rightleftharpoons B_2O_2$ to be greater than 99.6 kcal/mole. At 1500°K, they measured: $P_{B_2O_2} = 3.1 \times 10^{-5}$ atm, $P_{B_2O_3} = 5.3 \times 10^{-6}$ atm, and

$P_{BO} < 2 \times 10^{-6}$atm. Scheer[2] determined the molecular weight and vapor pressure of gaseous boric oxide effusing through two orifices by measuring the weight loss and the exerted force. His molecular weight confirmed the formula B_2O_3, and his vapor pressure at 1500°K was about 3×10^{-6} atm. Meschi, Chupka, and Berkowitz[3] analyzed the vapors effusing from a Knudsen cell containing B_2O_3 and water vapor. The main vapor species formed was HBO_2. For the reaction $1/2\ H_2O\ (g) + 1/2\ B_2O_3\ (s) \rightleftharpoons HBO_2$ (g), they measured $\Delta H_0^o = 47.6 \pm 2$ kcal/mole. They also identified the trimer $(HBO_2)_3$ and orthoboric acid vapor, H_3BO_3, in trace amounts equal to about 1 percent of the HBO_2.

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2. Spectroscopic Studies

a. Boron Monoxide (BO)

The structure of the simplest boron oxide, the diatomic molecule BO, was well known 30 years ago from the analysis of its emission spectrum. Herzberg's tabulation[1] gives the internuclear distance, the reduced mass, the dissociation energy, the vibrational and rotational constants, the electronic energy levels and the symmetries, angular momenta, and multiplicities of the electronic states, all of which have been deduced from the emission spectrum. Some of these quantities are listed in table VB-1.

b. Boron Dioxide (BO_2)

Although the spectrum of the oxide BO_2 has been seen for many years in the green "fluctuation bands" of B_2O_3, it has not been recognized and analyzed until recently. The bands are easily seen usually in combination with BO bands, when boric acid is introduced into a flame.

Pearse and Gaydon[2] described the fluctuation bands as being "due probably to a polyatomic emitter, perhaps an oxide of boron such as B_2O_3." Soulen and others[3] obtained the bands without accompanying BO bands by heating B_2O_3 in a tube furnace. Since the intensity seemed to be directly related to the vapor pressure of B_2O_3 (g) and since BO appeared to be absent, they concluded that the bands originated in the B_2O_3 molecule.

Kaskan and Millikan,[4] however, came to a different conclusion, based on the chemistry of boron-containing flames. They stated that the green bands could not have come from B_2O_3 in their flames, but most likely came from BO_2 which was formed in the flame reaction $OH + HOBO \rightarrow HOH + OBO$.

Mal'tsev and others[5] ascribed the green bands to BO_2 on the basis of chemical effects on the emission intensity from a tube furnace. When B_2O_3 was heated in inert atmospheres, the bands appeared weakly. This they attributed to the dissociation of B_2O_3 vapor: $B_2O_3 \rightarrow BO + BO_2$. When oxygen was admitted to the furnace, the intensity of the bands increased strongly. To explain this, they wrote $B_2O_3 + 1/2\ O_2 \rightarrow 2BO_2$. When B_2O_3 was heated in the presence of hydrogen, the fluctuation bands did not appear; perhaps this was due to the reaction $BO_2 + 1/2\ H_2 \rightarrow HBO_2$.

Kaskan and others show that the concentration of the substance responsible for the green bands depends on the fourth root of the pressure of the oxygen in equilibrium with the heated B_2O_3. This is just what is predicted by the equation $B_2O_3 + 1/2\ O_2 \rightarrow 2BO_2$.

Finally, Johns[7] has convincingly shown that the green bands are due to BO_2, and he has obtained structural data and vibration frequencies of the ground state and two excited electronic states of the molecule. Johns has obtained the electronic absorption spectrum when BCl_3-O_2 mixtures have been subjected to flash photolysis. His structural data for the ground state are given in table VB-1.

c. Metaboric Acid (HBO_2)

HBO_2, metaboric acid, is the principal vapor species which exists in equilibrium with water vapor and liquid B_2O_3 at high temperature.[8] The infrared emission bands which have been observed by Dows and Porter[9] and assigned to B_2O_3 were most likely due to HBO_2 because the tube in which the B_2O_3 was vaporized was open to the atmosphere.

White and others,[10] and Mal'tsev and others[5] have also reported features of the infrared spectrum of HBO_2. White has used his observed spectrum to calculate the frequencies of the normal modes of vibration of an HBO_2 molecule of an assumed molecular symmetry, and from the frequencies, he has calculated thermodynamic functions of the gaseous molecule. The molecule and its spectrum will be discussed in more detail in a subsequent section of this report.

d. Boric Anhydride (B_2O_3)

B_2O_3, boric anhydride, has been the subject of a number of different spectroscopic investigations, most of which appear to have obtained not the spectrum of B_2O_3 but the spectra of the products of its dissociation, reaction, or condensation. The erroneous assignment of the green "fluctuation bands" to B_2O_3 has already been mentioned. Also, it has been mentioned that the bands observed by Dows and Ported were more likely due to HBO_2 than to B_2O_3.

White and others[11] appear to have performed the most extensive study of the B_2O_3 spectrum to date. They observed the infrared emission spectrum of the B_2O_3 in a molybdenum tube which was heated by induction. Three principal emission bands were observed with wave numbers of approximately 2060, 1310, and 750 cm^{-1}. They have chosen a C_{2V} symmetry for the molecule (V-shape) and have assigned the bands to the antisymmetric fundamental vibrations as follows:

The 2060 cm^{-1} band was assigned to the ν_6 normal mode, essentially a B=O stretch; 1310 cm^{-1} was assigned to ν_7, a B-O stretch, and the 750 cm^{-1} band was assigned to ν_8, a B-O-B bending mode. From the assignments, they calculated the force constants and vibration frequencies of the nine normal modes of vibration, and also calculated the thermodynamic functions $(F° - H_0^\circ/T)$, $(H° - H_0^\circ/T)$, $S°$, and C_p.

Tatevskii and others[12] subsequently published an analysis of the vibrational spectrum of B_2O_3, in which they stated that the 1310 and 750 wave-number bands of White and others could not possibly have been due to the vibrations of the gaseous molecule as assigned, and that they were due to condensed-phase B_2O_3 in the light path. They stated that no reasonable choice of force constants could give a calculated value of 1300 cm^{-1} for the B-O stretching mode and suggested that the band should instead be near 900 cm^{-1}.

Tatevskii's analysis and criticism appear to be well founded. White and other investigators who have used the spectroscopic technique have always had interference from condensates formed in their optical path, and the 1300 cm^{-1} band is the strongest band in the spectra of condensed-phase borates, boric acid, and boric anhydride, while a band in the vicinity of 750 cm^{-1} is the next strongest. The bonding is of an entirely different type in the condensed phase, and qualitatively one can predict that the condensed and vapor-phase spectra will not be similar but different. Thus, there appears to be a strong possibility that White's analysis and thermodynamic calculations are erroneous in some respects. The same possibility of erroneous vibrational assignments and thermodynamic calculations exists in the case of the HBO_2 gaseous molecule.

Further support for the claim that the B-O stretching frequency should not be at 1300 cm^{-1} would appear to be given by Weltner and Warn,[13] who isolated B_2O_3 molecules at low temperature in matrices of argon and xenon and recorded the infrared absorption spectra. They observed a strong band at about 2130 cm^{-1}, a strong band at about 480 cm^{-1}, a medium strength band at 1240 cm^{-1}, and nothing at 1300 cm^{-1}.

e. Boron Oxide (B_2O_2)

B_2O_2 was also studied by White and others,[11] who observed an emission band at 1890 cm^{-1}. By assigning this band to the B-O stretching vibration, assuming the molecule to be linear, drawing certain analogies with vibrational spectrum of the molecule C_2N_2, and assuming a value of the B-B stretching force constant, they were able to calculate a vibrational spectrum and thermodynamic functions for B_2O_2. Weltner and Warn[13] also observed a band at about 1900 cm^{-1} from B_2O_2, their band being isolated in a matrix of inert gas at low temperature.

A brief summary of some of the properties of the boron oxides and hydroxides is given in table VB-1.

TABLE VB-1

SOME PROPERTIES OF BORON OXIDE VAPORS

Gaseous Compound	Conditions of Formation	Molecular Properties Which Appear to Be Reasonably Well Established	Remarks
BO	Forms in electric discharges through boron-containing compounds and oxygen. Also forms in the thermal decomposition of B_2O_3 at high temperatures	Equilibrium internuclear distance = 1.205Å; Dissociation energy = 9.1 eV; Fundamental vibration frequency = 1862 cm^{-1}; Stretching force constant = 13.3 x 10^5 dyne/cm	Molecular properties obtained from analysis of electronic emission spectrum.[1]
BO_2	Forms in photolysis of BCl_3-O_2 mixtures; forms in flame-reaction $HO + HBO_2 \rightarrow H_2O + BO_2$; forms in thermal decomposition of B_2O_3 at high temperatures	B-O bond distance = 1.265 Å; Fundamental vibration frequencies: ν_1 = 1070 cm^{-1}, ν_2 = 464 cm^{-1}, ν_3 = 1322 cm^{-1}; Stretching force constant = 10.8 x 10^5 dyne/cm	Molecular properties obtained from analysis of electronic absorption spectrum.[7]
HBO_2	Forms in reaction of water vapor with anhydrous liquid B_2O_3; distills out of orthoboric acid at high temperature; forms in boron-containing flames in air; is most prominent vapor species in boron-oxygen-water equilibrium at temperatures below the boiling point of B_2O_3	Infrared spectrum contains bands due to OH group and B=O group. B=O frequency not far from B=O frequency in B_2O_3	Only reported spectrum[10] suspected of being erroneous; hence, thermodynamic calculations based on spectrum may be incorrect
B_2O_2	Forms in reduction of B_2O_3 by B and in reduction of MgO by B	Molecule has B=O group or groups	One infrared band reported at 1890 cm^{-1} and assigned to B=O stretching in a linear symmetrical molecule.[11]
B_2O_3	Forms on dehydration of orthoboric acid in absence of reducing agents	Molecule contains B=O group or groups with absorption near 2000 cm^{-1}	Correct spectrum not firmly established.[11,12]

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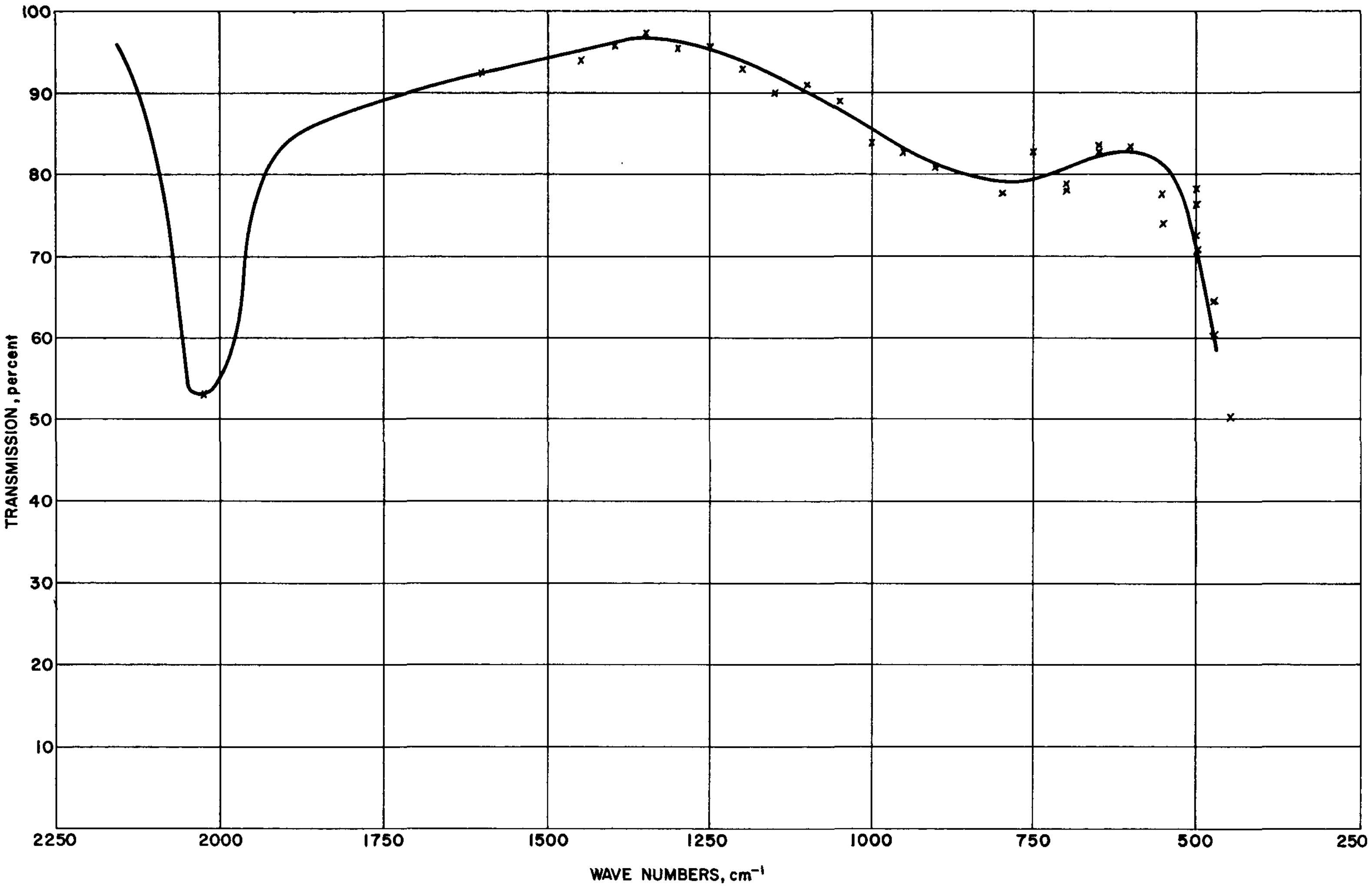

Figure V-1 INFRARED ABSORPTION SPECTRUM OF METABORIC ACID VAPOR [$HBO_2(g)$] FOR A PATH LENGTH OF 120 feet, A TEMPERATURE OF 1435°K, AND WATER VAPOR PRESSURE OF 2 cm Hg--B_2O_3 IN A PLATINUM BOAT -- NaCl PRISM
62-10096

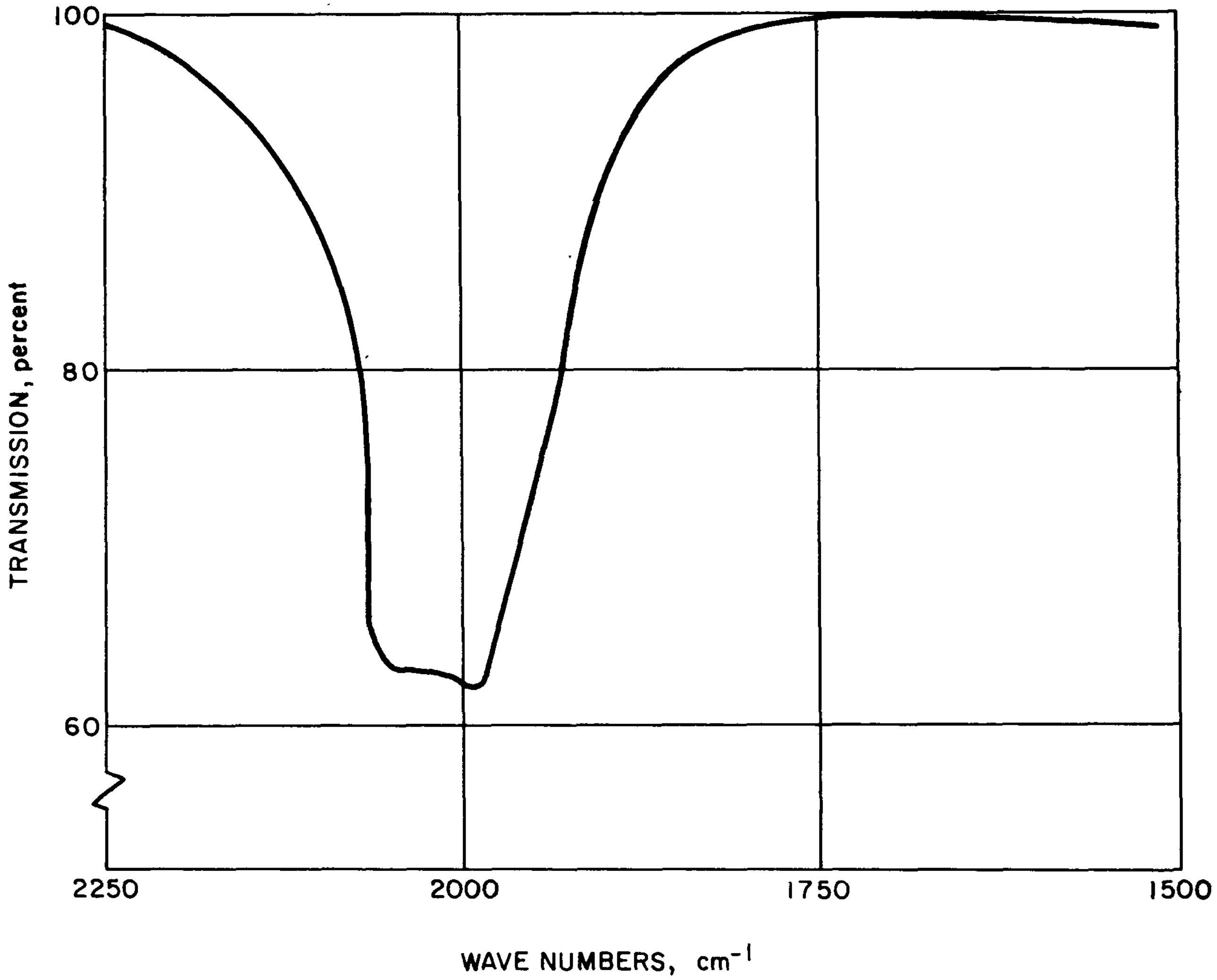

Figure V-2 INFRARED SPECTRUM OF METABORIC ACID VAPOR OBTAINED DURING DEHYDRATION OF B_2O_3 AT 1370°K FOR A PATH LENGTH OF 120 feet--CaF_2 PRISM
62-10095

C. EXPERIMENTAL RESULTS

It is an objective of the present experimental research program to obtain the the correct infrared spectra of boron oxides and hydroxides, and thus, to help settle some of the discrepancies and conflicts which exist regarding these spectra and their interpretation in terms of molecular structure and vibration frequencies. The spectrum of HBO_2 has been obtained and does indeed have certain features of interest, as will be discussed. Work is continuing on obtaining the spectra of B_2O_3 and B_2O_2 and further details of the spectrum of HBO_2.

The apparatus used was described in the first quarterly report. To obtain the spectrum of HBO_2, boric anyhdride was heated to 1435°K in a platinum-lined quartz boat in the presence of about 20 mm Hg pressure of water vapor. The optical path through the heated zone was approximately 120 feet. Although the design of the experiment suppressed particulate formation, it was considered necessary to take extra precautions to ensure avoiding false bands due to particulates or gaseous impurities. The spectrum was not scanned, but was plotted point by point, using the old-fashioned "sample in--sample out" technique. The method was as follows:

The vapors were put into the light path by raising the furnace temperature to the desired value; then with the monochromator set at a fixed wavelength, the output signal of the detector was observed. The furnace power was then cut off, and as the tube cooled the vapors condensed· then if there had been vapor absorption at the particular wavelength under study, a change in output signal was observed. Absorptions by vapor disappeared at a fast rate which could be calculated from the cooling curve and the Clausius-Clapeyron equation. It was not necessary actually to make the calculation because the strong B=O band at 2000 cm^{-1} was free from interference, and therefore, gave the correct rate of disappearance. All other true vapor bands were expected to disappear at the same rate as the 2000 cm^{-1} band.

The spectrum of figure V-1 was plotted by attributing to vapor absorption the difference between the output signal at the moment the power was cut off and the output signal 5 seconds later. Approximately three-fourths of the total change in output signal occurred in the first 5 seconds. All the points marked x in figure V-1 were obtained in this manner. The only place that the spectrum was scanned was in the vicinity of the 2000 cm^{-1} band. Absorption by particles disappeared at a slow rate, and thus was distinguishable from the true absorption bands of the vapors.

The 2000 cm^{-1} band has also been studied under conditions of better resolution, and the result is shown in figure V-2. The band is wide and flat on the bottom. Except for this flatness, it does not appear that there is resolvable structure because atmospheric water bands which are considerably narrower than the

HBO_2 band have been observed. The spectrum of figure V-2 has been obtained during the vacuum dehydration of orthoboric acid without added water vapor, and therefore, the intensity cannot be compared with the intensity of the corresponding band in figure V-1 which has been recorded under different conditions.

D. DISCUSSION OF RESULTS

Perhaps the most significant aspect of figure V-1 is the absence of any absorption band in the vicinity of 1400 cm^{-1}. Care has been taken to establish this point because condensed phase metaborates have a strong band in this region, and White and others[1] have reported a 1400 cm^{-1} band in metaboric acid vapor.

The absence of a 1400 cm^{-1} band in the vapor probably is to be expected on the basis of Tatevskii's argument that a reasonable assignment of bond-stretching force constants would give a value of about 900 cm^{-1} for the B-O stretching vibration in B_2O_3. The frequency should not be too much different in HBO_2.

If the absence of the 1400 cm^{-1} band is proved, the calculation of Tatevskii for B_2O_3 is supported. This indicates that the published interpretation of the HBO_2 vibrational spectrum[1] and the thermodynamic calculations based thereon are in need of revision.

It is interesting, and also, it may be instructive, to make a comparison of the set of molecules HBO_2, BO_2, and BO with the corresponding set of molecules in which nitrogen replaces boron; i. e., HNO_2, NO_2, and NO. The difference of two electrons between the boron atom and the nitrogen atom does, of course, lead to some significant differences in the chemical and physical properties of the two series of compounds.

Consider, for example, the boiling points; the boron-containing compounds exist in the vapor state only at very high temperatures; e. g., 1500°K, whereas the nitrogen-containing series exist as a vapor at room temperature. There is, however, a similarity in the equilibria which exist among the various gaseous molecules listed above, in that each acid gives water and the sesquioxide which, in turn, is in equilibrium with its dissociation products:

$$2\,HBO_2 \rightleftharpoons (B_2O_3 \rightleftharpoons BO + BO_2) + H_2O \quad , \qquad \text{(VD-1)}$$

$$2\,HNO_2 \rightleftharpoons (N_2O_3 \rightleftharpoons NO + NO_2) + H_2O \quad . \qquad \text{(VD-2)}$$

The main differences between the two sets of equilibria are (1) the different temperature ranges at which they exist, and (2) the dissociation of B_2O_3 proceeds to only a slight extent except at the very highest temperature, whereas the dissociation of N_2O_3 goes so far at room temperature that N_2O_3 cannot be detected spectroscopically.

There is still another similarity between the two sets of compounds; i. e., the existence of derivatives of the acids; e. g., analogous nitrites and metaborates exist in the condensed phase, and nitrites (such as CH_3 ONO) and metaborates (such as NaOBO) also exist in the vapor phase.

In some ways, the differences produced by the two electrons are not as great as the differences which can be produced by one electron because, in some compounds, the two extra electrons can be relegated to an unused "lone-pair" orbital. For example, metaboric acid and **nitrous** acid which have the two-electron difference exist and have similar molecular structures; however, there is no corresponding carbon-containing compound which would differ from each of the other two by one electron. Nor is there any known compound C_2O_3 analogous to B_2O_3 and N_2O_3.

A comparison of the spectra of metaboric acid and nitrous acid reveals a number of similarities. Listed below are frequencies published for nitrous acid by Jones, Badger, and Moore.[2]

Nitrous Acid Vapor

Functional Group	Frequency
	cm^{-1}
O-H stretch (cis)	3590
O-H stretch (trans)	3420
N=O stretch (trans) (N=O stretch in cis isomer obscured by band of NO_2)	1690
N-O stretch (cis)	856
N-O stretch (trans)	794
O-N-O bend (cis and trans)	600

Similar bands in the spectra of alkyl nitrites are listed by Tarte.[3]

Methyl Nitrite Vapor

Functional Group	Frequency
	cm^{-1}
N=O stretch (trans)	1681
N=O stretch (cis)	1625
N-O stretch (cis)	844
N-O stretch (trans)	814
O-N-O bend (cis)	617
O-N-O bend (trans)	565

Since definite assignments to functional groups seem clear cut in the case of nitrous acid, similar assignments should be possible for the HOBO molecule. From figure V-1, it seems reasonable to ascribe 2050 cm^{-1} to B=O stretching, 700 cm^{-1} to 900 cm^{-1} to B-O stretching, and 450 cm^{-1} to O-B-O bending. There should also be an OH frequency as reported by White and others.[1]

The last point to be discussed at present is the possibility of cis-trans isomerism in metaboric acid. It has been shown by Jones and others[2] and Tarte[3] that this type of isomerism is very pronounced in nitrous acid and in alkyl nitrites. Since both the O-N=O group and the R-O-N group are bent, stable cis and trans configurations are able to form. The effect on the infrared spectrum is a doubling of most of the bands, as shown in the listings above.

In the alkyl nitrites, the doubled N=O band is not resolved, and the resulting band has a flat bottom very similar in appearance to the flat bottom on the B=O band of HOBO in figure V-2. The shape of the band in figure V-2 therefore may be interpreted as evidence of cis-trans isomerism in HOBO which, in turn, means that the O-B=O group is not linear.

White and others[1] have assumed a linear O-B=O group, but they do not cite any particular reason for the assumption. It seems possible to obtain some support for assuming a bent O-B=O group by drawing an analogy between the behavior of the ONO angle, when H is added to form nitrous acid, and the possible behavior of the OBO angle, when H is added to form metaboric acid. Since the ONO angle decreases from about 140° in NO_2[4] to 116° in HONO[2], it may seem reasonable for the OBO angle to decrease from 180° in BO_2[4] to some lesser value in HOBO.

It will be of interest to obtain the OH band of metaboric acid with good resolution because if cis-trans isomerism does exist, the OH band will possibly be more split than the B=O band. An attempt to obtain the OH band is now underway.

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VI. COMPILATION OF THERMODYNAMIC TABLES

The thermodynamic tables (see tables VI-1 to VI-27) pertinent to this project are presented at the end of this section. A brief summary of basic data has been provided following each table to make it independent of the text as far as use of the table is concerned. However, for the details concerning the choice of data or methods of preparation of the tables, one should consult the main body of this report.

The order in which the tables are placed is according to the modified Hill[1] indexing system for chemical compounds as used by the JANAF Thermochemical Panel Compilation,[2] Chemical Abstracts, and the Classification Division of the U. S. Patent Office. In the upper right-hand corner of each table is an alphabetic arrangement of the atomic symbols in the chemical formula. The order of the tables is alphabetic according to this compound symbol except for carbon compounds which include the very large organic category. In carbon compounds, the elemental symbol "C" always comes first, immediately followed by "H" if hydrogen is present. The other elemental symbols in carbon compounds then follow in their regular order. The numbers of atoms of the elements in the compound play a secondary role in determining the tables' positions. Their influence is subordinate to the order in which the atomic symbols occur in the compound symbol. For example, any compound symbol containing "C_2" would come after all others containing "C," regardless of any other element symbols the compound symbol might contain. Reference-state and condensed-phase tables have been placed before ideal gas tables.

Solid lines with double entries have been used to designate primary transitions, such as solid-state changes, melting points, and normal boiling points, in reference-state and condensed-phase tables. Dotted lines have been used in the corresponding places in ideal gas tables to indicate discontinuities in the heats of formation of the gases due to the primary transitions in the reference-state phases. Since primary transitions in condensed phases of compounds are not reflected as discontinuities in heats of formation of the corresponding ideal gases, double entries have not been included at such temperatures in ideal gas tables of compounds. Double entries with no lines have been used in tables of compounds to indicate discontinuities in heats of formation due to transitions in the elements.

REFERENCES FOR SECTION VI

1. Hill, E. A., J. Am. Chem. Soc. 22, 478 (1900).

2. Dergazarian, T. E. et al, JANAF Interim Thermochemical Tables, Vols. 1 and 2, Dow Chem. Co., Midland, Mich. (31 December 1960).

THE THERMODYNAMIC TABLES

TABLE	TITLE	FILING ORDER
	Calcium Oxide	CaO
VI-1	Condensed Phases	
VI-2	Ideal Molecular Gas	
	Cerium	Ce
VI-3	Reference State	
VI-4	Ideal Monatomic Gas	
	Cerium Oxide	CeO
VI-5	Ideal Molecular Gas	
	Magnesium Oxide	MgO
VI-6	Condensed Phases	
VI-7	Ideal Molecular Gas	
	Manganese	Mn
VI-8	Reference State	
VI-9	Ideal Monatomic Gas	
	Manganese Oxide	MnO
VI-10	Ideal Molecular Gas	
	Platinum Monoxide	OPt
VI-11	Ideal Molecular Gas	
	Rhenium Oxide	ORe
VI-12	Ideal Molecular Gas	
	Rhodium Monoxide	ORh
VI-13	Ideal Molecular Gas	
	Strontium Oxide	OSr
VI-14	Condensed Phases	
VI-15	Ideal Molecular Gas	
	Technetium Monoxide	OTc
VI-16	Ideal Molecular Gas	
	Thorium Monoxide	OTh
VI-17	Ideal Molecular Gas	
	Platinum	Pt
VI-18	Reference State	
VI-19	Ideal Monatomic Gas	
	Rhenium	Re
VI-20	Reference State	
VI-21	Ideal Monatomic Gas	

THE THERMODYNAMIC TABLES (Concl'd)

TABLE	TITLE	FILING ORDER
	Rhodium	Rh
VI-22	Reference State	
VI-23	Ideal Monatomic Gas	
	Technetium	Tc
VI-24	Reference State	
VI-25	Ideal Monatomic Gas	
	Thorium	Th
VI-26	Reference State	
VI-27	Ideal Monatomic Gas	

TABLE VI - 1

CALCIUM OXIDE CONDENSED PHASES CaO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ca from 0° to 1123°K, Liquid Ca from 1123° to 1765°K Gaseous Ca from 1765°K to 4000°K, Gaseous O_2, Solid CaO from 0° to 2860°K, Liquid CaO from 2860° to 4000°K.

	cal/°K gfw			Kcal/gfw			
T,°K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-1.668	-150.666	-150.666	Infinite
298.15	10.230	9.561	9.561	0.000	-151.410	-143.988	105.541
300	10.254	9.624	9.561	0.019	-151.410	-143.942	104.857
400	11.120	12.708	9.976	1.093	-151.336	-141.463	77.288
500	11.579	15.243	10.784	2.230	-151.248	-139.005	60.756
600	11.878	17.383	11.710	3.404	-151.171	-136.564	49.741
700	12.101	19.231	12.655	4.603	-151.115	-134.184	41.877
737	12.172	19.856	13.001	5.052	-151.101	-133.237	39.508
737	12.172	19.856	13.001	5.052	-151.341	-133.237	39.508
800	12.283	20.859	13.581	5.822	-151.319	-131.690	35.974
900	12.442	22.315	14.472	7.059	-151.333	-129.236	31.381
1000	12.587	23.634	15.323	8.310	-151.408	-126.778	27.706
1100	12.722	24.840	16.134	9.576	-151.547	-124.309	24.697
1123	12.752	25.103	16.315	9.869	-151.588	-123.739	24.080
1123	12.752	25.103	16.315	9.869	-153.658	-123.739	24.080
1200	12.851	25.952	16.907	10.855	-153.569	-121.690	22.162
1300	12.975	26.986	17.643	12.146	-153.447	-119.039	20.011
1400	13.095	27.952	18.345	13.449	-153.315	-116.397	18.170
1500	13.214	28.859	19.016	14.765	-153.175	-113.765	16.575
1600	13.330	29.716	19.658	16.092	-153.026	-111.142	15.181
1700	13.445	30.527	20.274	17.431	-152.869	-108.529	13.952
1764.79	13.519	31.033	20.661	18.307	-152.762	-106.843	13.229
1764.79	13.519	31.033	20.661	18.307	-188.633	-106.843	13.229
1800	13.559	31.299	20.865	18.781	-188.489	-105.219	12.775
1900	13.672	32.035	21.434	20.143	-188.073	-100.605	11.572
2000	13.784	32.739	21.982	21.515	-187.651	-96.011	10.491
2100	13.896	33.415	22.510	22.899	-187.222	-91.439	9.516
2200	14.007	34.064	23.021	24.295	-186.787	-86.888	8.631
2300	14.118	34.689	23.514	25.701	-186.347	-82.359	7.826
2400	14.228	35.292	23.993	27.118	-185.902	-77.845	7.088
2500	14.338	35.875	24.456	28.546	-185.457	-73.354	6.412
2600	14.448	36.439	24.906	29.986	-185.009	-68.878	5.789
2700	14.558	36.987	25.344	31.436	-184.563	-64.422	5.214
2800	14.667	37.518	25.769	32.897	-184.117	-59.979	4.681
2860	14.733	37.830	26.019	33.779	-183.852	-57.327	4.380
2860	16.500	43.844	26.019	50.979	-166.652	-57.327	4.380
2900	16.500	44.073	26.266	51.639	-166.407	-55.793	4.204
3000	16.500	44.632	26.869	53.289	-165.805	-51.989	3.787
3100	16.500	45.173	27.451	54.939	-165.222	-48.203	3.398
3200	16.500	45.697	28.013	56.589	-164.659	-44.442	3.035
3300	16.500	46.205	28.557	58.239	-164.117	-40.690	2.695
3400	16.500	46.697	29.083	59.889	-163.601	-36.961	2.376
3500	16.500	47.176	29.593	61.539	-163.110	-33.242	2.076
3600	16.500	47.641	30.088	63.189	-162.647	-29.537	1.793
3700	16.500	48.093	30.569	64.839	-162.214	-25.845	1.527
3800	16.500	48.533	31.035	66.489	-161.810	-22.164	1.275
3900	16.500	48.961	31.490	68.139	-161.440	-18.495	1.036
4000	16.500	49.379	31.932	69.789	-161.102	-14.835	0.810

CALCIUM OXIDE CONDENSED PHASES

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T,°K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± .200	± .150	± .150	± .000	± .500	± .570	± .420
1000	± .430	± .290	± .210	± .080	± .760	± .870	± .190
2000	± .930	± .460	± .300	± .330	± 1.700	± 1.540	± .170
2860	± 1.740	± .610	± .370	± .680	± 2.050	± 1.860	± .140
2860	± 1.000	± 1.100	± .370	± 2.080	± 3.450	± 1.860	± .140
4000	± 2.000	± 1.600	± .650	± 3.790	± 5.160	± 3.320	± .180

Summary of Basic Data

Solid has a face-centered cubic (NaCl type) structure.

m.p.	b.p.
$T_m = 2860^\circ \pm 30^\circ K$	Decomposes at
$\Delta H_m = 17.200 \pm 1.400$ Kcal/gfw	1 atm. at 3890°K
$\Delta S_m = 6.000 \pm .500$ e.u./gfw	

$S_{298}^\circ = 9.561 \pm .150$ e.u./gfw

$H_{298}^\circ - H_0^\circ = 1668$ cal/gfw

$\Delta H_{f298}^\circ = -151.410 \pm .500$ Kcal/gfw

gfw = 56.08

Solid heat capacity from Kelley, K. K., Bureau of Mines Bull. 584 (1960).

C_p° (liquid) assumed to be 16.500 ± 2.000 cal/°K gfw

TABLE VI - 2

CALCIUM OXIDE IDEAL MOLECULAR GAS CaO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid Ca from 0° to 1123°K, Liquid Ca from 1123° to 1765°K, Gaseous Ca from 1765° to 6000°K; Gaseous O_2, Gaseous CaO.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-2.117	1.095	1.095	Infinite
298.15	7.553	54.217	54.217	0.000	0.800	-5.092	3.733
300	7.561	54.263	54.217	0.014	0.795	-5.129	3.736
400	7.952	56.495	54.518	0.791	0.572	-7.070	3.863
500	8.233	58.301	55.100	1.601	0.333	-8.953	3.913
600	8.427	59.820	55.763	2.434	0.069	-10.786	3.928
700	8.564	61.130	56.439	3.284	-0.224	-12.573	3.925
737	8.604	61.572	56.685	3.602	-0.341	-13.222	3.921
737	8.604	61.572	56.685	3.602	-0.581	-13.222	3.921
800	8.663	62.281	57.099	4.146	-0.786	-14.295	3.905
900	8.737	63.305	57.732	5.016	-1.165	-15.960	3.875
1000	8.795	64.229	58.337	5.892	-1.617	-17.582	3.842
1100	8.841	65.069	58.911	6.774	-2.139	-19.153	3.805
1123	8.850	65.253	59.039	6.978	-2.269	-19.508	3.796
1123	8.850	65.253	59.039	6.978	-4.339	-19.508	3.796
1200	8.879	65.840	59.457	7.660	-4.554	-20.540	3.741
1300	8.911	66.552	59.976	8.550	-4.833	-21.862	3.675
1400	8.938	67.214	60.469	9.442	-5.113	-23.161	3.615
1500	8.963	67.831	60.940	10.337	-5.393	-24.441	3.561
1600	8.985	68.411	61.389	11.235	-5.673	-25.702	3.511
1700	9.005	68.956	61.818	12.134	-5.956	-26.944	3.464
1764.79	9.017	69.294	62.087	12.720	-6.139	-27.750	3.436
1764.79	9.017	69.294	62.087	12.720	-42.010	-27.750	3.436
1800	9.023	69.471	62.229	13.036	-42.024	-27.465	3.334
1900	9.041	69.960	62.623	13.939	-42.067	-26.654	3.066
2000	9.058	70.424	63.002	14.844	-42.112	-25.842	2.824
2100	9.075	70.866	63.366	15.750	-42.161	-25.027	2.604
2200	9.091	71.289	63.717	16.659	-42.213	-24.211	2.405
2300	9.108	71.694	64.055	17.569	-42.269	-23.393	2.223
2400	9.125	72.082	64.382	18.480	-42.331	-22.570	2.055
2500	9.142	72.455	64.697	19.394	-42.399	-21.746	1.901
2600	9.161	72.814	65.003	20.309	-42.476	-20.919	1.758
2700	9.180	73.160	65.299	21.226	-42.563	-20.091	1.626
2800	9.200	73.495	65.586	22.145	-42.660	-19.256	1.503
2900	9.221	73.818	65.865	23.066	-42.771	-18.420	1.388
3000	9.244	74.132	66.135	23.989	-42.895	-17.577	1.280
3100	9.268	74.436	66.399	24.915	-43.036	-16.732	1.180
3200	9.293	74.731	66.655	25.843	-43.195	-15.886	1.085
3300	9.320	75.017	66.904	26.773	-43.374	-15.027	0.995
3400	9.349	75.297	67.147	27.707	-43.574	-14.169	0.911
3500	9.378	75.568	67.385	28.643	-43.797	-13.303	0.831
3600	9.410	75.834	67.616	29.583	-44.044	-12.428	0.754
3700	9.443	76.092	67.842	30.525	-44.318	-11.547	0.682
3800	9.477	76.345	68.063	31.471	-44.619	-10.659	0.613
3900	9.513	76.593	68.280	32.421	-44.948	-9.767	0.547
4000	9.551	76.835	68.491	33.374	-45.307	-8.862	0.484
4100	9.590	77.072	68.698	34.331	-45.696	-7.945	0.424
4200	9.630	77.304	68.901	35.292	-46.117	-7.025	0.366
4300	9.672	77.532	69.100	36.257	-46.569	-6.093	0.310
4400	9.714	77.756	69.295	37.227	-47.052	-5.144	0.256
4500	9.758	77.975	69.486	38.200	-47.568	-4.191	0.204
4600	9.803	78.191	69.674	39.179	-48.115	-3.225	0.153
4700	9.849	78.404	69.859	40.161	-48.697	-2.250	0.105
4800	9.896	78.613	70.040	41.149	-49.308	-1.257	0.057
4900	9.944	78.818	70.218	42.141	-49.952	-0.256	0.011
5000	9.993	79.021	70.393	43.138	-50.628	0.760	-0.033
5100	10.042	79.220	70.566	44.140	-51.336	1.789	-0.077
5200	10.092	79.417	70.735	45.147	-52.074	2.833	-0.119
5300	10.142	79.611	70.902	46.159	-52.845	3.887	-0.160
5400	10.193	79.803	71.067	47.176	-53.648	4.958	-0.201
5500	10.244	79.992	71.229	48.198	-54.483	6.044	-0.240
5600	10.296	80.178	71.388	49.225	-55.350	7.148	-0.279
5700	10.348	80.363	71.546	50.258	-56.252	8.261	-0.317
5800	10.400	80.545	71.701	51.296	-57.190	9.398	-0.354
5900	10.453	80.725	71.854	52.339	-58.164	10.547	-0.391
6000	10.505	80.903	72.005	53.387	-59.179	11.714	-0.427

CALCIUM OXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

S^{o}_{298} = 54.217 e.u./gfw $H^{o}_{298} - H^{o}_{0}$ = 2117 cal/gfw

ΔH^{o}_{f298} = 0.800 ± 15.000 Kcal/gfw D_0 = 100 Kcal/gfw   gfw = 56.08

Spectroscopic constants from Hultin, M. and A. Lagerqvist, Ark. Fys 2, 471 (1950) and Lagerqvist, A. Ark. Fys. 8, 83 (1954). Ground state assumed to be ${}^1\Sigma$. Spectroscopic constants (in units of cm^{-1}) which were assumed and/or estimated are:

State	E	ω_e	$\omega_e x_e$	B_e	α_e	$D_e \times 10^6$
$X\ {}^3\Sigma$	0	850.0	5.0	0.53	0.004	0.7
$X\ {}^1\Sigma$	15000					
${}^3\Sigma$	20000	725.0	4.0	0.45	0.003	0.7

TABLE VI - 3

CERIUM REFERENCE STATE Ce

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid from 0° to 1077°K,
Liquid from 1077° to 4271°K, Gas from 4271° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-2.133			
298.15	6.440	17.640	17.640	0.000			
300	6.446	17.680	17.640	0.012			
400	6.759	19.576	17.897	0.672			
500	7.096	21.120	18.391	1.364			
600	7.456	22.446	18.959	2.092			
700	7.840	23.623	19.543	2.856			
800	8.248	24.697	20.121	3.661			
900	8.680	25.693	20.685	4.507			
1000	9.135	26.631	21.233	5.397			
1003	9.149	26.658	21.250	5.425			
1003	9.047	27.356	21.250	6.125			
1077	9.047	28.000	21.692	6.794			
1077	9.345	29.149	21.692	8.032			
1100	9.345	29.347	21.850	8.247			
1200	9.345	30.160	22.509	9.182			
1300	9.345	30.908	23.126	10.116			
1400	9.345	31.601	23.707	11.051			
1500	9.345	32.245	24.255	11.985			
1600	9.345	32.849	24.774	12.920			
1700	9.345	33.415	25.266	13.854			
1800	9.345	33.949	25.733	14.789			
1900	9.345	34.455	26.179	15.723			
2000	9.345	34.934	26.605	16.658			
2100	9.345	35.390	27.013	17.592			
2200	9.345	35.825	27.403	18.527			
2300	9.345	36.240	27.779	19.461			
2400	9.345	36.638	28.139	20.396			
2500	9.345	37.019	28.487	21.330			
2600	9.345	37.386	28.822	22.265			
2700	9.345	37.738	29.146	23.199			
2800	9.345	38.078	29.459	24.134			
2900	9.345	38.406	29.762	25.068			
3000	9.345	38.723	30.055	26.003			
3100	9.345	39.029	30.340	26.937			
3200	9.345	39.326	30.616	27.872			
3300	9.345	39.614	30.884	28.806			
3400	9.345	39.893	31.145	29.741			
3500	9.345	40.163	31.399	30.675			
3600	9.345	40.427	31.646	31.610			
3700	9.345	40.683	31.887	32.544			
3800	9.345	40.932	32.122	33.479			
3900	9.345	41.175	32.351	34.413			
4000	9.345	41.411	32.574	35.348			
4100	9.345	41.642	32.793	36.282			
4200	9.345	41.867	33.006	37.217			
4270.73	9.345	42.023	33.154	37.880			
4270.73	8.202	62.396	33.154	124.889			
4300	8.216	62.452	33.352	125.127			
4400	8.264	62.641	34.016	125.951			
4500	8.312	62.828	34.655	126.780			
4600	8.360	63.011	35.269	127.614			
4700	8.407	63.191	35.860	128.452			
4800	8.453	63.369	36.433	129.295			
4900	8.498	63.543	36.984	130.142			
5000	8.542	63.715	37.516	130.994			
5100	8.584	63.885	38.032	131.851			
5200	8.624	64.052	38.531	132.711			
5300	8.663	64.217	39.014	133.576			
5400	8.699	64.379	39.482	134.444			
5500	8.734	64.539	39.936	135.315			
5600	8.766	64.697	40.377	136.190			
5700	8.795	64.852	40.805	137.068			
5800	8.822	65.005	41.221	137.949			
5900	8.846	65.156	41.625	138.833			
6000	8.868	65.305	42.019	139.718			

CERIUM REFERENCE STATE

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
298.15	± .050	± .800	± .800	± .000			
1003	± .050	± .830	± .810	± .020			
1003	± .050	± .838	± .810	± .028			
1077	± .050	± .840	± .810	± .030			
1077	± .050	± .844	± .810	± .034			
2000	± .100	± .900	± .840	± .110			
3000	± 1.000	± 1.120	± .900	± .660			
4000	± 2.900	± 1.680	± 1.030	± 2.610			
4270.73	± 3.400	± 1.890	± 1.080	± 3.460			
4270.73	± .300	± .770	± .660	± .490			
5000	± .400	± .830	± .680	± .750			
6000	± .500	± .910	± .710	± 1.200			

Summary of Basic Data

Structure of solid is complicated and uncertain; probably face-centered cubic (α-Ce) below 150°K, hexagonal close packed (β-Ce) between 150° and 260°K, face-centered cubic (γ-Ce) between 260° and 1003°K, and body-centered cubic (δ-Ce) between 1003°K and m.p.

$T_t(IV) = 1003^\circ \pm 5^\circ K$ m.p. $= 1077^\circ \pm 9^\circ K$ b.p. $= 4271 \pm 490^\circ K$

$\Delta H_t(IV) = 700 \pm 8$ cal/gfw $\Delta H_m = 1238 \pm 4$ cal/gfw $\Delta H_v = 87.009 \pm 6.450$ Kcal/gfw

$\Delta S_t(IV) = 0.698 \pm .008$ e.u./gfw $\Delta S_m = 1.149 \pm .004$ e.u./gfw $\Delta S_v = 20.373 \pm 2.836$ e.u./gfw

$S_{298}^o = 17.640 \pm .800$ e.u./gfw $H_{298}^o - H_0^o = 2133$ cal/gfw gfw = 140.13

$C_p^o(\gamma) = 5.649 + 2.300 \times 10^{-3}T + 11.862 \times 10^{-7}T^2$ (cal/°K gfw)

$C_p^o(\delta) = 9.047$ cal/°K gfw

$C_p^o(\ell) = 9.345$ cal/°K gfw

TABLE VI - 4

CERIUM IDEAL MONATOMIC GAS Ce

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid from 0° to 1077°K,
Liquid from 1077° to 4271°K, Gas from 4271° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-1.509	95.624	95.624	Infinite
298.15	5.438	43.591	43.591	0.000	95.000	87.263	-63.962
300	5.447	43.625	43.591	0.010	94.998	87.215	-63.533
400	5.894	45.255	43.810	0.577	94.905	84.635	-46.240
500	6.219	46.608	44.238	1.185	94.821	82.076	-35.874
600	6.455	47.763	44.732	1.819	94.727	79.536	-28.970
700	6.666	48.774	45.239	2.475	94.619	77.013	-24.043
800	6.874	49.678	45.738	3.152	94.491	74.506	-20.353
900	7.073	50.449	46.222	3.849	94.342	72.017	-17.487
1000	7.248	51.254	46.688	4.566	94.169	69.545	-15.198
1003	7.253	51.275	46.702	4.588	94.163	69.472	-15.137
1003	7.253	51.275	46.702	4.588	93.463	69.472	-15.137
1077	7.361	51.796	47.034	5.128	93.334	67.707	-13.739
1077	7.361	51.796	47.034	5.128	92.096	67.707	-13.739
1100	7.391	51.952	47.135	5.298	92.051	67.186	-13.348
1200	7.497	52.599	47.564	6.043	91.861	64.934	-11.826
1300	7.571	53.202	47.975	6.796	91.680	62.696	-10.540
1400	7.618	53.766	48.368	7.556	91.505	60.475	-9.440
1500	7.645	54.292	48.746	8.319	91.334	58.264	-8.489
1600	7.657	54.786	49.108	9.084	91.164	56.066	-7.658
1700	7.660	55.250	49.456	9.850	90.996	53.877	-6.926
1800	7.658	55.688	49.790	10.616	90.827	51.697	-6.277
1900	7.653	56.102	50.112	11.382	90.659	49.527	-5.697
2000	7.648	56.494	50.421	12.147	90.489	47.368	-5.176
2100	7.644	56.867	50.719	12.911	90.319	45.217	-4.706
2200	7.641	57.223	51.007	13.676	90.149	43.071	-4.279
2300	7.640	57.563	51.284	14.440	89.979	40.938	-3.890
2400	7.642	57.888	51.553	15.204	89.808	38.806	-3.534
2500	7.647	58.200	51.813	15.968	89.638	36.685	-3.207
2600	7.655	58.500	52.064	16.733	89.468	34.571	-2.906
2700	7.666	58.789	52.308	17.499	89.300	32.463	-2.628
2800	7.680	59.068	52.544	18.267	89.133	30.362	-2.370
2900	7.698	59.338	52.774	19.036	88.968	28.265	-2.130
3000	7.718	59.599	52.997	19.806	88.803	26.174	-1.907
3100	7.742	59.853	53.214	20.579	88.642	24.091	-1.698
3200	7.769	60.099	53.425	21.355	88.483	22.011	-1.503
3300	7.799	60.338	53.631	22.133	88.327	19.935	-1.320
3400	7.832	60.572	53.832	22.915	88.174	17.864	-1.148
3500	7.867	60.799	54.028	23.700	88.025	15.798	-0.986
3600	7.905	61.021	54.219	24.488	87.878	13.737	-0.834
3700	7,945	61.239	54.406	25.281	87.737	11.680	-0.690
3800	7.987	61.451	54.588	26.077	87.598	9.629	-0.554
3900	8.030	61.659	54.767	26.878	87.465	7.578	-0.425
4000	8.075	61.863	54.942	27.683	87.335	5.528	-0.302
4100	8.122	62.063	55.113	28.493	87.211	3.488	-0.186
4200	8.169	62.259	55.281	29.308	87.091	1.445	-0.075
4270.73	8.202	62.396	55.398	29.889	87.009	0.000	0.000
4270.73	8.202	62.396	55.398	29.889			
4300	8.216	62.452	55.446	30.127			
4400	8.264	62.641	55.607	30.951			
4500	8.312	62.828	55.765	31.780			
4600	8.360	63.011	55.921	32.614			
4700	8.407	63.191	56.074	33.452			
4800	8.453	63.369	56.224	34.295			
4900	8.498	63.543	56.371	35.142			
5000	8.542	63.715	56.517	35.994			
5100	8.584	63.885	56.659	36.851			
5200	8.624	64.052	56.800	37.711			
5300	8.663	64.217	56.938	38.576			
5400	8.699	64.379	57.075	39.444			
5500	8.734	64.539	57.209	40.315			
5600	8.766	64.697	57.341	41.190			
5700	8.795	64.852	57.472	42.068			
5800	8.822	65.005	57.600	42.949			
5900	8.846	65.156	57.727	43.833			
6000	8.868	65.305	57.852	44.718			

CERIUM IDEAL MONATOMIC GAS

Summary of Uncertainty Estimates

T °K	cal/°K gfw			Kcal/gfw			
	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
298 15	± 200	± 500	± 500	± 000	± 2 500	± 2 890	± 2 120
1003	± 150	± 590	± 540	± 050	± 2 570	± 3 850	± 840
1003	± 150	± 590	± 540	± 050	± 2 580	± 3 850	± 840
1077	± 150	± 600	± 540	± 060	± 2 590	± 3 950	± 800
1077	± 150	± 600	± 540	± 060	± 2 600	± 3 950	± 800
2000	± 100	± 670	± 590	± 170	± 2 780	± 5 360	± 590
3000	± 100	± 710	± 620	± 270	± 3 430	± 7 060	± 510
4000	± 200	± 760	± 650	± 420	± 5 530	± 9 220	± 500
4270 73	± 300	± 770	± 660	± 490	± 6 450	± 9 930	± 510
4270 73	± 300	± 770	± 660	± 490			
5000	± 400	± 830	± 680	± 750			
6000	± 500	± 910	± 710	± 1 200			

Summary of Basic Data

S^o_{298} 43 591 ± 500 e u /gfw

H^o_{298} H^o_0 1509 cal gfw

ΔH^o_{f298} 95 000 ± 2 500 Kcal/gfw

gfw 140 13

Spectroscopic data not available energy levels assumed to be the same as those of lanthanum

TABLE VI - 5

CERIUM OXIDE IDEAL MOLECULAR GAS CeO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ce from 0° to 1077°K, Liquid Ce from 1077° to 4271°K, Gaseous Ce from 4271° to 6000°K, Gaseous O_2, Gaseous CeO.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-2.114	-30.044	-30.044	Infinite
298.15	7.521	57.219	57.219	0.000	-31.100	-35.595	26.090
300	7.529	57.266	57.200	0.014	-31.105	-35.617	25.946
400	7.915	59.487	57.520	0.787	-31.347	-37.092	20.265
500	8.196	61.285	58.099	1.593	-31.598	-38.501	16.828
600	8.391	62.798	58.759	2.423	-31.874	-39.855	14.516
700	8.528	64.103	59.432	3.270	-32.180	-41.162	12.851
800	8.626	65.248	60.088	4.128	-32.526	-42.421	11.588
900	8.699	66.269	60.719	4.994	-32.913	-43.636	10.596
1000	8.755	67.188	61.321	5.867	-33.344	-44.805	9.792
1003	8.756	67.213	61.338	5.893	-33.358	-44.838	9.769
1003	8.756	67.213	61.338	5.893	-34.058	-44.838	9.769
1077	8.789	67.837	61.763	6.543	-34.387	-45.621	9.257
1077	8.789	67.837	61.763	6.543	-35.625	-45.621	9.257
1100	8.799	68.025	61.893	6.745	-35.735	-45.834	9.106
1200	8.834	68.792	62.436	7.626	-36.213	-46.731	8.510
1300	8.864	69.500	62.953	8.511	-36.691	-47.590	8.000
1400	8.889	70.158	63.444	9.399	-37.170	-48.410	7.557
1500	8.911	70.772	63.913	10.289	-37.649	-49.197	7.168
1600	8.933	71.348	64.360	11.181	-38.130	-49.950	6.823
1700	8.954	71.890	64.787	12.076	-38.611	-50.674	6.514
1800	8.975	72.402	65.196	12.972	-39.094	-51.371	6.237
1900	8.999	72.888	65.588	13.871	-39.576	-52.039	5.986
2000	9.025	73.351	65.965	14.772	-40.060	-52.682	5.757
2100	9.054	73.792	66.327	15.676	-40.543	-53.300	5.547
2200	9.087	74.214	66.676	16.583	-41.027	-53.897	5.354
2300	9.125	74.618	67.013	17.493	-41.509	-54.471	5.176
2400	9.167	75.008	67.338	18.408	-41.990	-55.027	5.011
2500	9.215	75.383	67.652	19.327	-42.469	-55.559	4.857
2600	9.268	75.745	67.957	20.251	-42.946	-56.074	4.713
2700	9.325	76.096	68.252	21.181	-43.419	-56.570	4.579
2800	9.387	76.437	68.538	22.116	-43.889	-57.048	4.453
2900	9.454	76.767	68.816	23.058	-44.356	-57.509	4.334
3000	9.525	77.089	69.087	24.007	-44.817	-57.958	4.222
3100	9.600	77.403	69.350	24.963	-45.274	-58.385	4.116
3200	9.678	77.709	69.607	25.927	-45.726	-58.804	4.016
3300	9.759	78.008	69.857	26.899	-46.171	-59.206	3.921
3400	9.842	78.301	70.101	27.879	-46.610	-59.594	3.830
3500	9.926	78.588	70.340	28.868	-47.043	-59.970	3.745
3600	10.012	78.869	70.573	29.864	-47.471	-60.334	3.663
3700	10.098	79.144	70.801	30.870	-47.889	-60.685	3.584
3800	10.184	79.415	71.024	31.884	-48.303	-61.023	3.509
3900	10.270	79.681	71.243	32.907	-48.708	-61.354	3.438
4000	10.355	79.942	71.458	33.938	-49.108	-61.678	3.370
4100	10.439	80.199	71.668	34.978	-49.500	-61.985	3.304
4200	10.521	80.452	71.874	36.026	-49.887	-62.285	3.241
4270.73	10.578	80.629	72.018	36.775	-50.157	-62.494	3.198
4270.73	10.578	80.629	72.018	36.775	-137.166	-62.494	3.198
4300	10.601	80.701	72.077	37.082	-137.243	-61.987	3.150
4400	10.679	80.945	72.276	38.146	-137.507	-60.232	2.992
4500	10.754	81.187	72.472	39.217	-137.770	-58.474	2.840
4600	10.827	81.424	72.664	40.296	-138.033	-56.708	2.694
4700	10.896	81.658	72.853	41.382	-138.296	-54.943	2.555
4800	10.963	81.888	73.039	42.475	-138.559	-53.158	2.420
4900	11.026	82.115	73.223	43.575	-138.823	-51.384	2.292
5000	11.087	82.339	73.403	44.680	-139.090	-49.600	2.168
5100	11.144	82.560	73.581	45.792	-139.360	-47.808	2.049
5200	11.197	82.777	73.756	46.909	-139.633	-46.008	1.934
5300	11.247	82.991	73.929	48.031	-139.913	-44.210	1.823
5400	11.295	83.202	74.099	49.158	-140.198	-42.402	1.716
5500	11.338	83.410	74.267	50.289	-140.490	-40.590	1.613
5600	11.379	83.616	74.432	51.425	-140.792	-38.769	1.513
5700	11.417	83.818	74.596	52.565	-141.107	-36.948	1.417
5800	11.451	84.017	74.757	53.708	-141.437	-35.116	1.323
5900	11.483	84.214	74.916	54.854	-141.785	-33.283	1.233
6000	11.512	84.407	75.073	56.004	-142.153	-31.436	1.145

CERIUM OXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

S^o_{298} = 57.219 e.u./gfw

$H^o_{298}-H^o_0$ = 2114 cal/gfw

ΔH^o_{f298} = -31.100 ± 5.000 Kcal/gfw

gfw = 156.13

Vibrational spectroscopic constants from Herzberg, G., Molecular Spectra and Molecular Structure. I. Spectra of Diatomic Molecules, 2nd Ed. van Nostrand, New York (1950).
Assumed and/or estimated molecular properties (in units of cm^{-1}):

State	B_e	$D_e x10^7$	g	E
X	0.359	2.5	2	-
A	0.326	2.2	2	-
B	0.327	2.3	2	-
X'	0.349	2.3	2	13720.0
D	0.329	2.3	2	34276.0
E	0.335	2.3	2	34584.0

$r_o = 1.81Å$

TABLE VI - 6

MAGNESIUM OXIDE CONDENSED PHASES MgO

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid Mg from 0° to 923°K, Liquid Mg from 923° to 1377°K, Gaseous Mg from 1377° to 4000°K; Gaseous O_2; Solid MgO from 0° to 3098°K, Liquid MgO from 3098° to 4000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
0	0.000	0.000	Infinite	-1.235	-142.703	-142.703	Infinite
298.15	8.906	6.439	6.439	0.000	-143.700	-135.988	99.677
300	8.939	6.495	6.440	0.017	-142.701	-135.941	99.028
400	10.148	9.252	6.807	0.978	-143.704	-133.351	72.856
500	10.854	11.599	7.538	2.031	-143.650	-130.770	57.157
600	11.323	13.622	8.387	3.141	-143.583	-128.199	46.694
700	11.656	15.393	9.263	4.291	-143.519	-125.640	39.225
800	11.905	16.967	10.130	5.469	-143.471	-123.090	33.625
900	12.098	18.381	10.970	6.670	-143.440	-120.544	29.271
923	12.135	18.683	11.154	6.949	-143.436	-119.955	28.402
923	12.135	18.683	11.154	6.949	-145.563	-119.955	28.402
1000	12.251	19.663	11.775	7.888	-145.545	-117.824	25.749
1100	12.375	20.837	12.547	9.119	-145.513	-115.054	22.858
1200	12.478	21.918	13.283	10.362	-145.474	-112.286	20.449
1300	12.565	22.921	13.987	11.614	-145.431	-109.524	18.412
1376.37	12.622	23.644	14.505	12.584	-145.394	-107.401	17.045
1376.37	12.622	23.644	14.505	12.584	-176.134	-107.401	17.045
1400	12.638	23.855	14.659	12.874	-176.058	-106.251	16.586
1500	12.701	24.729	15.301	14.141	-175.723	-101.276	14.755
1600	12.756	25.550	15.916	15.414	-175.385	-96.325	13.157
1700	12.804	26.325	16.506	16.692	-175.046	-91.393	11.749
1800	12.845	27.058	17.072	17.975	-174.703	-86.481	10.500
1900	12.882	27.754	17.616	19.261	-174.361	-81.590	9.385
2000	12.915	28.415	18.139	20.551	-174.018	-76.716	8.383
2100	12.945	29.046	18.644	21.844	-173.675	-71.860	7.478
2200	12.971	29.649	19.131	23.140	-173.332	-67.020	6.658
2300	12.994	30.226	19.601	24.438	-172.989	-62.196	5.910
2400	13.016	30.780	20.055	25.739	-172.646	-57.385	5.225
2500	13.035	31.311	20.494	27.042	-172.305	-52.589	4.597
2600	13.052	31.823	20.921	28.346	-171.965	-47.808	4.018
2700	13.068	32.316	21.334	29.652	-171.627	-43.040	3.484
2800	13.082	32.791	21.734	30.959	-171.290	-38.283	2.988
2900	13.095	33.251	22.124	32.268	-170.955	-33.539	2.527
3000	13.107	33.695	22.502	33.578	-170.623	-28.807	2.099
3098	13.118	34.116	22.863	34.863	-170.300	-24.178	1.706
3098	14.600	40.088	22.863	53.363	-151.800	-24.178	1.706
3100	14.600	40.097	22.874	53.392	-151.790	-24.094	1.699
3200	14.600	40.561	23.420	54.852	-151.316	-19.986	1.365
3300	14.600	41.010	23.946	56.312	-150.846	-15.891	1.052
3400	14.600	41.446	24.454	57.772	-150.381	-11.802	0.759
3500	14.600	41.869	24.946	59.232	-149.921	-7.737	0.483
3600	14.600	42.280	25.421	60.692	-149.467	-3.676	0.223
3700	14.600	42.680	25.882	62.152	-149.017	0.367	-0.022
3800	14.600	43.069	26.329	63.612	-148.576	4.399	-0.253
3900	14.600	43.449	26.764	65.072	-148.140	8.418	-0.472
4000	14.600	43.819	27.186	66.532	-147.712	12.426	-0.679

MAGNESIUM OXIDE CONDENSED PHASES

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± .050	± .020	± .020	± .000	± .500	± .510	± .370
923	—	—	—	—	± .610	± .580	± .140
923	—	—	—	—	± .640	± .580	± .140
1000	± .280	± .160	± .080	± .080	—	—	—
1376.37	—	—	—	—	± .900	± .760	± .120
1376.37	—	—	—	—	± 1.350	± .760	± .120
2000	± .940	± .390	± .180	± .410	± 1.560	± 1.000	± .110
3098	± 1.780	± .570	± .290	± .860	± 2.010	± 1.620	± .110
3098	± 1.000	± 1.050	± .290	± 2.360	± 3.510	± 1.620	± .110
4000	± 2.000	± 1.440	± .500	± 3.750	± 4.900	± 2.820	± .150

Summary of Basic Data

Solid has face-centered cubic (NaCl type) structure.

m. p.

$T_m = 3098° \pm 20°K$

$\Delta H_m = 18.500 \pm 1.500$ Kcal/gfw

$\Delta S_m = 5.972 \pm .480$ e.u. /gfw

b. p.

Decomposes at 1 atm pressure at 3110°K

$S_{298}^\circ = 6.439 \pm .020$ e.u. /gfw

$\Delta H_{f298}^\circ = -143.700 \pm .500$ Kcal/gfw

C_p° (solid) $= 13.7146 - 4.494 \times 10^{-5} T - 1418 T^{-1}$

$H_{298}^\circ - H_0^\circ = 1235$ cal/gfw

gfw = 40.32

C_p°(liquid) = 14.600 cal/°K gfw

TABLE VI - 7

MAGNESIUM OXIDE IDEAL MOLECULAR GAS MgO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mg from 0° to 923°K, Liquid Mg from 923° to 1377°K, Gaseous Mg from 3177° to 6000°K, Gaseous O_2, Gaseous MgO.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-2.112	-10.980	-10.980	Infinite
298.15	7.506	52.891	52.891	0.000	-11.100	-17.238	12.635
300	7.514	52.938	52.891	0.014	-11.104	-17.276	12.585
400	7.912	55.156	53.191	0.786	-11.296	-19.305	10.547
500	8.211	56.955	53.770	1.593	-11.488	-21.286	9.303
600	8.425	58.472	54.430	2.425	-11.699	-23.225	8.459
700	8.581	59.783	55.103	3.276	-11.934	-25.128	7.845
800	8.698	60.937	55.762	4.140	-12.200	-26.996	7.375
900	8.789	61.967	56.395	5.015	-12.495	-28.827	7.000
923	8.807	62.189	56.537	5.217	-12.568	-29.244	6.924
923	8.807	62.189	56.537	5.217	-14.695	-29.244	6.924
1000	8.862	62.897	57.000	5.897	-14.936	-30.449	6.654
1100	8.924	63.744	57.575	6.787	-15.245	-31.985	6.355
1200	8.977	64.523	58.122	7.682	-15.554	-33.493	6.100
1300	9.023	65.244	58.642	8.582	-15.863	-34.975	5.880
1376.37	9.056	65.764	59.026	9.278	-16.100	-36.106	5.730
1376.37	9.056	65.764	59.026	9.278	-46.840	-36.106	5.730
1400	9.066	65.914	59.138	9.486	-46.846	-35.922	5.607
1500	9.105	66.541	59.611	10 395	-46.869	-35.141	5.120
1600	9.141	67.130	60.063	11.307	-46.892	-34.360	4.693
1700	9.176	67.686	60.496	12.223	-46.915	-33.576	4.316
1800	9.210	68.211	60.910	13.142	-46.936	-32.789	3.981
1900	9.243	68.711	61.308	14.065	-46.957	-32.005	3.681
2000	9.275	69.186	61.690	14.991	-46.978	-31.218	3.411
2100	9.306	69.640	62.059	15.920	-46.999	-30.432	3.167
2200	9.338	70.074	62.414	16.852	-47.020	-29.643	2.945
2300	9.369	70.490	62.757	17.788	-47.039	-28.855	2.742
2400	9.401	70.890	63.088	18.726	-47.059	-28.064	2.555
2500	9.433	71.276	63.409	19.668	-47.079	-27.276	2.384
2600	9.465	71.647	63.719	20.613	-47.098	-26.483	2.226
2700	9.498	72.006	64.021	21.561	-47.118	-25.695	2.080
2800	9.531	72.353	64.313	22.512	-47.137	-24.904	1.944
2900	9.565	72.689	64.597	23.467	-47.156	-24.111	1.817
3000	9.600	73.016	64.874	24.425	-47.176	-23.324	1.699
3100	9.636	73.333	65.143	25.387	-47.195	-22.528	1.588
3200	9.673	73.641	65.405	26.353	-47.215	-21.738	1.485
3300	9.711	73.941	65.661	27.322	-47.236	-20.950	1.387
3400	9.750	74.233	65.911	28.295	-47.258	-20.156	1.296
3500	9.791	74.518	66.155	29.272	-47.281	-19.369	1.209
3600	9.833	74.797	66.393	30.253	-47.306	-18.575	1.128
3700	9.876	75.069	66.626	31.238	-47.331	-17.786	1.051
3800	9.921	75.335	66.854	32.228	-47.360	-16.996	0.977
3900	9.967	75.596	67.078	33.222	-47.390	-16.207	0.908
4000	10.014	75.852	67.297	34.221	-47.423	-15.418	0.842
4100	10.064	76.103	67.511	35.225	-47.460	-14.630	0.780
4200	10.114	76.349	67.722	36.234	-47.500	-13.843	0.720
4300	10.167	76.591	67.929	37.248	-47.544	-13.052	0.663
4400	10.220	76.829	68.132	38.267	-47.594	-12.266	0.609
4500	10.276	77.063	68.332	39.292	-47.647	-11.483	0.558
4600	10.332	77.293	68.528	40.322	-47.707	-10.695	0.508
4700	10.391	77.520	68.721	41.359	-47.772	-9.906	0.461
4800	10.450	77.744	68.911	42.400	-47.846	-9.120	0.415
4900	10.511	77.965	69.098	43.448	-47.927	-8.334	0.372
5000	10.573	78.182	69.282	44.502	-48.016	-7.545	0.330
5100	10.637	78.397	69.464	45.563	-48.115	-6.770	0.290
5200	10.701	78.610	69.643	46.629	-48.226	-5.978	0.251
5300	10.767	78.820	69.819	47.702	-48.349	-5.188	0.214
5400	10.834	79.027	69.993	48.782	-48.485	-4.404	0.178
5500	10.901	79.232	70.165	49.868	-48.637	-3.617	0.144
5600	10.970	79.436	70.335	50.962	-48.807	-2.832	0.111
5700	11.039	79.637	70.503	52.062	-48.996	-2.043	0.078
5800	11.110	79.836	70.669	53.168	-49.212	-1.260	0.047
5900	11.181	80.033	70.833	54.282	-49.453	-0.462	0.017
6000	11.252	80.229	70.995	55.403	-49.725	0.324	-0.012

MAGNESIUM OXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

S^{o}_{298} = 52 891 e.u /gfw

$H^{o}_{298} - H^{o}_{0}$ = 2112 cal/gfw

ΔH^{o}_{f298} = -11.100 ± 15.000 Kcal/gfw

gfw = 40.32

Spectroscopic constants from the vibrational analysis of Brewer, L. and R. F. Porter. J. Chem. Phys., 22, 1876 (1954). Low-lying $^1\Sigma$ state taken as 19,200 cm^{-1} above ground $^3\Sigma$ state. Values of B_e s for triplet states estimated from B_e/ω_e of singlet states.

TABLE VI - 8

MANGANESE — REFERENCE STATE — Mn

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid from 0° to 1517°K, Liquid from 1517° to 2319°K, Gas from 2319° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-1.194			
298.15	6.290	7.640	7.640	0.000			
300	6.301	7.679	7.640	0.012			
400	6.822	9.567	7.894	0.669			
500	7.244	11.135	8.390	1.373			
600	7.628	12.490	8.963	2.117			
700	7.993	13.694	9.554	2.898			
800	8.349	14.785	10.141	3.715			
900	8.700	15.788	10.713	4.568			
990	9.012	16.632	11.213	5.365			
990	8.983	17.168	11.213	5.896			
1000	8.990	17.259	11.273	5.985			
1100	9.056	18.119	11.857	6.888			
1200	9.122	18.909	12.412	7.797			
1300	9.188	19.642	12.941	8.712			
1374	9.237	20.152	13.315	9.394			
1374	10.700	20.552	13.315	9.943			
1400	10.700	20.752	13.452	10.221			
1410	10.700	20.829	13.504	10.328			
1410	11.300	21.138	13.504	10.764			
1500	11.300	21.837	13.983	11.781			
1517	11.300	21.964	14.072	11.973			
1517	11.000	24.272	14.072	15.473			
1600	11.000	24.857	14.616	16.386			
1700	11.000	25.524	15.238	17.486			
1800	11.000	26.153	15.827	18.586			
1900	11.000	26.748	16.387	19.686			
2000	11.000	27.312	16.919	20.786			
2100	11.000	27.849	17.427	21.886			
2200	11.000	28.360	17.912	22.986			
2300	11.000	28.849	18.377	24.086			
2318.80	11.000	28.939	18.463	24.295			
2318.80	5.006	51.688	18.463	77.048			
2400	5.018	51.861	19.588	77.454			
2500	5.040	52.066	20.884	77.956			
2600	5.067	52.264	22.086	78.462			
2700	5.101	52.456	23.208	78.970			
2800	5.142	52.642	24.255	79.482			
2900	5.193	52.824	25.238	79.999			
3000	5.253	53.001	26.161	80.521			
3100	5.322	53.174	27.029	81.050			
3200	5.403	53.344	27.848	81.586			
3300	5.495	53.512	28.624	82.131			
3400	5.598	53.677	29.358	82.685			
3500	5.713	53.841	30.055	83.251			
3600	5.841	54.004	30.718	83.828			
3700	5.981	54.166	31.350	84.419			
3800	6.133	54.327	31.952	85.025			
3900	6.297	54.489	32.528	85.646			
4000	6.473	54.650	33.079	86.285			
4100	6.661	54.813	33.608	86.941			
4200	6.859	54.975	34.114	87.617			
4300	7.068	55.139	34.601	88.313			
4400	7.287	55.304	35.070	89.031			
4500	7.515	55.471	35.522	89.771			
4600	7.751	55.638	35.957	90.534			
4700	7.995	55.808	36.377	91.322			
4800	8.244	55.979	36.785	92.134			
4900	8.500	56.151	37.178	92.971			
5000	8.759	56.325	37.558	93.834			
5100	9.022	56.502	37.927	94.723			
5200	9.288	56.679	38.287	95.638			
5300	9.554	56.859	38.636	96.580			
5400	9.821	57.040	38.975	97.549			
5500	10.088	57.222	39.305	98.545			
5600	10.352	57.407	39.627	99.567			
5800	10.873	57.779	40.246	101.689			
6000	11.376	58.156	40.837	103.914			

MANGANESE REFERENCE STATE

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± .050	± .040	± .040	± .000			
990	± .050	± .070	± .050	± .020			
990	± .050	± .150	± 050	± .100			
1374	± .100	± .180	± .080	± .130			
1374	± .200	± .230	± .080	± .210			
1410	± .300	± .240	± 090	± .220			
1410	± .500	± 290	± .090	± .280			
1517	± .500	± .320	± .100	± .330			
1517	± .500	± .650	± .100	± 830			
2000	± 1.610	± .950	± .270	± 1.350			
2318.80	± 2.310	± 1.230	± .380	± 1.980			
2318.80	± .000	± .002	± .003	± .000			
3000	± .000	± .002	± .003	± .001			
4000	± .001	± .003	± .003	± .001			
5000	± .002	± .003	± .003	± .002			
6000	± .003	± .003	± .003	± .004			

Summary of Basic Data

Solid has four crystalline modifications

$$\alpha \overset{I}{\rightleftharpoons} \beta \overset{II}{\rightleftharpoons} \gamma \overset{III}{\rightleftharpoons} \delta$$

α-Mn is body-centered cubic, A1 type

β-Mn is primitive cubic, A13 type

γ-Mn is face-centered cubic, A1 type

δ-Mn is body-centered cubic, A2 type

Transition	I	II	III	m.p.	b.p.
Temperature (°K)	990 ± 15	1374 ± 10	1410 ± 5	1517 ± 3	2319 ± 50
ΔH (cal/gfw)	531 ± 80	549 ± 80	436 ± 60	3500 ± 50	52.753 ± 2,280
ΔS (e.u /gfw)	0.536 ± .080	0 400 ± .050	0.309 ± .050	2.308 ± 330	22 749 ± 1.506

$S_{298}^\circ = 7.640 \pm .040$ e.u./gfw $H_{298}^\circ - H_0^\circ = 1194$ cal/gfw gfw = 54.94

$C_p^\circ(\alpha\text{-Mn}) - 5.704 + 3.380\text{x}10^{-3}T - 0.375\text{x}10^{5}T^{-2}$ (cal/°K gfw)

$C_p^\circ(\beta\text{-Mn}) = 8\ 330 + 0.660\text{x}10^{-3}T$ (cal/°K gfw)

$C_p^\circ(\gamma\text{-Mn}) = 10.700$ cal/°K gfw $C_p^\circ(\text{liquid}) = 11.000$ cal/°K gfw

$C_p^\circ(\delta\text{-Mn}) = 11.300$ cal/°K gfw

TABLE VI - 9

MANGANESE — IDEAL MONATOMIC GAS — Mn

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid from 0° to 1517°K, Liquid from 1517° to 2319°K, Gas from 2319° to 6000°K

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-1.481	66.713	66.713	Infinite
298.15	4.968	41.494	41.494	0.000	67.000	56.907	-41.712
300	4.968	41.525	41.494	0.009	66.997	56.844	-41.409
400	4.968	42.954	41.689	0.506	66.837	53.482	-29.220
500	4.968	44.063	42.057	1.003	66.630	50.167	-21.927
600	4.968	44.968	42.469	1.500	66.383	46.896	-17.081
700	4.968	45.734	42.882	1.996	66.098	43.670	-13.634
800	4.968	46.398	43.281	2.493	65.778	40.488	-11.060
900	4.968	46.983	43.660	2.990	65.422	37.348	-9.060
990	4.968	47.457	43.985	3.437	65.072	34.556	-7.628
990	4.968	47.457	43.985	3.437	64.541	34.556	-7.628
1000	4.968	47.506	44.019	3.487	64.502	34.254	-7.486
1100	4.968	47.980	44.358	3.984	64.096	31.249	-6.208
1200	4.968	48.412	44.678	4.481	63.684	28.281	-5.150
1300	4.968	48.810	44.981	4.977	63.265	25.348	-4.261
1374	4.968	49.085	45.195	5.345	62.951	23.197	-3.690
1374	4.968	49.085	45.195	5.345	62.402	23.197	-3.690
1400	4.968	49.178	45.268	5.474	62.253	22.458	-3.506
1410	4.968	49.213	45.295	5.524	62.196	22.175	-3.437
1410	4.968	49.213	45.295	5.524	61.760	22.175	-3.437
1500	4.968	49.521	45.540	5.971	61.190	19.664	-2.865
1517	4.968	49.577	45.586	6.055	61.082	19.193	-2.765
1517	4.968	49.577	45.586	6.055	57.582	19.193	-2.765
1600	4.969	49.841	45.799	6.468	57.082	17.107	-2.337
1700	4.969	50.143	46.046	6.965	56.479	14.626	-1.880
1800	4.971	50.427	46.281	7.462	55.876	12.183	-1.479
1900	4.973	50.695	46.507	7.959	55.273	9.772	-1.124
2000	4.977	50.951	46.722	8.456	54.670	7.394	-0.808
2100	4.982	51.194	46.930	8.954	54.068	5.044	-0.525
2200	4.991	51.426	47.129	9.453	53.467	2.723	-0.270
2300	5.002	51.648	47.320	9.953	52.867	0.431	-0.041
2318.80	5.005	51.652	65.529	17.753	52.753	0.000	0.000
2318.80	5.005	51.652	65.529	17.753			
2400	5.018	51.861	47.505	10.454			
2500	5.040	52.066	47.684	10.956			
2600	5.067	52.264	47.856	11.462			
2700	5.101	52.456	48.023	11.970			
2800	5.142	52.642	48.184	12.482			
2900	5.193	52.824	48.341	12.999			
3000	5.253	53.001	48.494	13.521			
3100	5.322	53.174	48.642	14.050			
3200	5.403	53.344	48.786	14.586			
3300	5.495	53.512	48.927	15.131			
3400	5.598	53.677	49.064	15.685			
3500	5.713	53.841	49.198	16.251			
3600	5.841	54.004	49.330	16.828			
3700	5.981	54.166	49.458	17.419			
3800	6.133	54.327	49.584	18.025			
3900	6.297	54.489	49.708	18.646			
4000	6.473	54.650	49.829	19.285			
4100	6.661	54.813	49.949	19.941			
4200	6.859	54.975	50.067	20.617			
4300	7.068	55.139	50.183	21.313			
4400	7.287	55.304	50.297	22.031			
4500	7.515	55.471	50.410	22.771			
4600	7.751	55.638	50.522	23.534			
4700	7.995	55.808	50.633	24.322			
4800	8.244	55.979	50.742	25.134			
4900	8.500	56.151	50.851	25.971			
5000	8.759	56.325	50.959	26.834			
5100	9.022	56.502	51.066	27.723			
5200	9.288	56.679	51.172	28.638			
5300	9.554	56.859	51.278	29.580			
5400	9.821	57.040	51.383	30.549			
5500	10.088	57.222	51.487	31.545			
5600	10.352	57.407	51.591	32.567			
5800	10.873	57.779	51.798	34.689			
6000	11.376	58.156	52.004	36.914			

MANGANESE IDEAL MONATOMIC GAS

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
298.15	± .000	± .002	± .002	± .000	± .300	± .310	
990	-	-	-	-	± .320	± .350	
990	-	-	-	-	± .400	± .350	
1000	± .000	± .002	± .002	± .000	-	-	
1374	-	-	-	-	± .430	± .410	
1374	-	-	-	-	± .510	± .410	
1410	-	-	-	-	± .520	± .430	
1410	-	-	-	-	± .580	± .430	
1517	-	-	-	-	± .630	± .450	
1517	-	-	-	-	± 1.130	± .450	
2000	± .000	± .002	± .003	± .000	± 1.650	± .840	
2318.80	-	-	-	-	± 2.280	± 1.180	
3000	± .000	± .002	± .003	± .001			
4000	± .001	± .003	± .003	± .001			
5000	± .002	± .003	± .003	± .002			
6000	± .003	± .003	± .003	± .004			

Summary of Basic Data

S_{298}^o = 41.494 ± .002 e.u. /gfw

$H_{298}^o - H_0^o$ = 1481 cal/gfw

ΔH_{f298}^o = 67.000 ± .300 Kcal/gfw

gfw = 54.94

Spectroscopic energy levels from Moore, C., Nat. Bur. Stds. Circular 467, Vol. 2 (15 August 1952).

TABLE VI - 10

MANGANESE OXIDE — IDEAL MOLECULAR GAS — MnO

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid Mn from 0° to 1517°K, Liquid Mn from 1517° to 2319°K, Gaseous Mn from 2319° to 6000°K; Gaseous O_2; Gaseous MnO.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
0	0.000	0.000	Infinite	-2.118	31.000	31.000	Infinite
298.15	7.569	55.616	55.616	0.000	30.600	23.602	-17.300
300	7.577	55.663	55.616	0.014	30.595	23.558	-17.161
400	7.968	57.899	55.918	0.792	30.361	21.247	-11.608
500	8.247	59.709	56.501	1.604	30.104	18.998	-8.304
600	8.439	61.231	57.166	2.439	29.817	16.803	-6.120
700	8.573	62.542	57.843	3.290	29.499	14.658	-4.576
800	8.671	63.694	58.503	4.152	29.144	12.563	-3.432
900	8.744	64.719	59.138	5.023	28.755	10.512	-2.553
990	8.795	65.554	59.683	5.812	28.375	8.706	-1.922
990	8.795	65.554	59.683	5.812	27.844	8.706	-1.922
1000	8.801	65.644	59.743	5.900	27.801	8.513	-1.861
1100	8.846	66.485	60.318	6.783	27.362	6.606	-1.312
1200	8.884	67.256	60.865	7.669	26.915	4.738	-0.863
1300	8.915	67.968	61.384	8.559	26.461	2.909	-0.489
1374	8.936	68.461	61.751	9.220	26.122	1.578	-0.251
1374	8.936	68.461	61.751	9.220	25.573	1.578	-0.251
1400	8.943	68.630	61.878	9.452	25.414	1.126	-0.176
1410	8.943	68.694	61.927	9.542	25.353	0.951	-0.147
1410	8.945	68.694	61.927	9.542	24.917	0.951	-0.147
1500	8.967	69.248	62.349	10.348	24.314	-0.559	0.081
1517	8.971	69.348	62.426	10.501	24.201	-0.838	0.121
1517	8.971	69.348	62.426	10.501	20.701	-0.838	0.121
1600	8.988	69.827	62.799	11.246	20.169	-2.006	0.274
1700	9.008	70.373	63.229	12.145	19.527	-3.373	0.434
1800	9.026	70.888	63.640	13.047	18.884	-4.701	0.571
1900	9.043	71.377	64.035	13.951	18.241	-5.993	0.689
2000	9.059	71.841	64.414	14.856	17.596	-7.252	0.792
2100	9.075	72.284	64.778	15.762	16.949	-8.478	0.882
2200	9.090	72.707	65.129	16.671	16.303	-9.674	0.961
2300	9.105	73.111	65.467	17.580	15.653	-10.840	1.030
2318.80	9.108	73.185	65.529	17.753	15.530	-11.057	1.042
2318.80	9.108	73.185	65.529	17.753	-37.223	-11.057	1.042
2400	9.119	73.499	65.794	18.491	-37.265	-10.144	0.924
2500	9.134	73.872	66.110	19.404	-37.318	-9.011	0.788
2600	9.149	74.231	66.416	20.318	-37.376	-7.881	0.662
2700	9.164	74.576	66.712	21.234	-37.436	-6.745	0.546
2800	9.179	74.910	66.999	22.151	-37.503	-5.610	0.438
2900	9.195	75.233	67.278	23.070	-37.575	-4.468	0.337
3000	9.211	75.545	67.549	23.990	-37.653	-3.326	0.242
3100	9.228	75.848	67.812	24.912	-37.738	-2.181	0.154
3200	9.246	76.142	68.068	25.836	-37.831	-1.037	0.071
3300	9.264	76.427	68.317	26.761	-37.934	0.118	-0.008
3400	9.282	76.704	68.560	27.689	-38.045	1.270	-0.082
3500	9.302	76.974	68.797	28.618	-38.169	2.427	-0.152
3600	9.322	77.237	69.029	29.549	-38.304	3.584	-0.218
3700	9.343	77.493	69.255	30.482	-38.452	4.748	-0.280
3800	9.364	77.743	69.475	31.418	-38.615	5.917	-0.340
3900	9.387	77.987	69.691	32.355	-38.793	7.089	-0.397
4000	9.410	78.226	69.902	33.295	-38.988	8.266	-0.452
4100	9.433	78.459	70.107	34.237	-39.200	9.456	-0.504
4200	9.458	78.688	70.311	35.182	-39.431	10.633	-0.553
4300	9.483	78.911	70.509	36.129	-39.682	11.826	-0.601
4400	9.509	79.130	70.703	37.079	-39.954	13.026	-0.647
4500	9.535	79.345	70.894	38.031	-40.247	14.229	-0.691
4600	9.562	79.556	71.081	38.987	-40.562	15.438	-0.733
4700	9.590	79.763	71.264	39.945	-40.903	16.655	-0.774
4800	9.618	79.967	71.445	40.905	-41.268	17.882	-0.814
4900	9.647	80.166	71.622	41.869	-41.658	19.112	-0.852
5000	9.677	80.363	71.796	42.836	-42.074	20.345	-0.889
5100	9.707	80.556	71.967	43.806	-42.518	21.588	-0.925
5200	9.738	80.746	72.135	44.779	-42.990	22.852	-0.960
5300	9.769	80.934	72.301	45.755	-43.492	24.115	-0.994
5400	9.801	81.118	72.464	46.734	-44.027	25.389	-1.027
5500	9.833	81.300	72.624	47.717	-44.592	26.676	-1.060
5600	9.865	81.479	72.782	48.703	-45.192	27.971	-1.092
5800	9.932	81.830	73.091	50.686	-46.499	30.591	-1.153
6000	10.001	82.172	73.392	52.683	-47.970	33.258	-1.211

MANGANESE OXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

$S^o_{298} = 55.616$ $H^o_{298} - H^o_0 = 2118$ cal/gfw

$\Delta H^o_{f298} = 30.600 \pm 10.000$ Kcal/gfw gfw = 70.94

Assumed and/or estimated molecular properties (in units of cm^{-1} and Å)

E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	$D_e(x10^7)$	r_e(Å)	g
0	839.55	4.79	-	0.499	7.1	1.65	4
17909.59	762.75	9.60	0.06	0.453	6.4	-	2

Vibrational constants from Das Sarma, J. M., Z. Physik 157, 98 (1959).

TABLE VI - 11

PLATINUM MONOXIDE IDEAL MOLECULAR GAS OPt

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid Pt from 0° to 2043°K, Liquid Pt from 2043° to 4108°K, Gaseous Pt from 4108° to 6000°K, Gaseous O_2, Gaseous PtO.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
0	0.000	0.000	Infinite	-2.125	88.797	88.797	Infinite
298.15	7.631	60.495	60.495	0.000	88.600	80.836	-59.251
300	7.639	60.543	60.496	0.014	88.597	80.787	-58.851
400	8.019	62.795	60.800	0.798	88.399	78.215	-42.733
500	8.276	64.614	61.387	1.614	88.209	75.691	-33.083
600	8.447	66.140	62.055	2.451	88.015	73.206	-26.664
700	8.562	67.451	62.735	3.301	87.813	70.753	-22.089
800	8.643	68.600	63.397	4.162	87.599	68.331	-18.666
900	8.701	69.621	64.033	5.029	87.370	65.936	-16.011
1000	8.744	70.540	64.639	5.902	87.127	63.567	-13.892
1100	8.777	71.375	65.214	6.778	86.869	61.223	-12.163
1200	8.802	72.140	65.760	7.657	86.598	58.903	-10.727
1300	8.822	72.846	66.278	8.538	86.312	56.606	-9.516
1400	8.838	73.500	66.771	9.421	86.012	54.332	-8.481
1500	8.851	74.110	67.240	10.306	85.697	52.082	-7.588
1600	8.862	74.682	67.687	11.191	85.367	49.852	-6.809
1700	8.871	75.219	68.115	12.078	85.024	47.640	-6.124
1800	8.879	75.727	68.524	12.965	84.664	45.453	-5.518
1900	8.885	76.207	68.916	13.854	84.292	43.284	-4.979
2000	8.891	76.663	69.292	14.742	83.903	41.136	-4.495
2043	8.893	76.852	69.449	15.125	83.732	40.276	-4.308
2043	8.893	76.852	69.449	15.125	79.034	40.276	-4.308
2100	8.895	77.097	69.653	15.632	78.797	39.140	-4.073
2200	8.900	77.511	70.001	16.521	78.381	37.260	-3.701
2300	8.903	77.906	70.336	17.412	77.964	35.400	-3.364
2400	8.906	78.285	70.659	18.302	77.543	33.560	-3.056
2500	8.909	78.649	70.972	19.193	77.120	31.734	-2.774
2600	8.912	78.998	71.274	20.084	76.695	29.927	-2.515
2700	8.914	79.335	71.566	20.975	76.267	28.138	-2.277
2800	8.916	79.659	71.849	21.867	75.838	26.364	-2.058
2900	8.918	79.972	72.124	22.758	75.405	24.604	-1.854
3000	8.919	80.274	72.391	23.650	74.971	22.859	-1.665
3100	8.921	80.567	72.650	24.542	74.534	21.130	-1.490
3200	8.922	80.850	72.902	25.434	74.095	19.414	-1.326
3300	8.923	81.125	73.147	26.327	73.655	17.713	-1.173
3400	8.924	81.391	73.385	27.219	73.213	16.025	-1.030
3500	8.926	81.650	73.618	28.112	72.769	14.349	-0.896
3600	8.926	81.901	73.844	29.004	72.322	12.689	-0.770
3700	8.927	82.146	74.065	29.897	71.874	11.037	-0.652
3800	8.928	82.384	74.281	30.790	71.425	9.398	-0.541
3900	8.929	82.616	74.492	31.683	70.973	7.771	-0.435
4000	8.930	82.842	74.698	32.575	70.519	6.158	-0.336
4100	8.930	83.062	74.899	33.468	70.064	4.554	-0.243
4108.34	8.930	83.079	74.915	33.539	70.024	4.639	-0.247
4108.34	8.930	83.079	74.915	33.539	-51.495	4.639	-0.247
4200	8.931	83.277	75.096	34.361	-51.667	5.671	-0.295
4300	8.931	83.488	75.289	35.255	-51.861	7.038	-0.358
4400	8.932	83.693	75.478	36.148	-52.060	8.410	-0.418
4500	8.932	83.894	75.662	37.041	-52.264	9.792	-0.476
4600	8.933	84.090	75.843	37.934	-52.471	11.173	-0.531
4700	8.933	84.282	76.021	38.827	-52.684	12.559	-0.584
4800	8.934	84.470	76.195	39.721	-52.901	13.948	-0.635
4900	8.934	84.654	76.366	40.614	-53.123	15.343	-0.684
5000	8.934	84.835	76.533	41.508	-53.351	16.745	-0.732
5100	8.935	85.012	76.698	42.401	-53.587	18.144	-0.777
5200	8.935	85.185	76.859	43.294	-53.829	19.560	-0.822
5300	8.935	85.356	77.018	44.188	-54.080	20.975	-0.865
5400	8.935	85.523	77.174	45.082	-54.340	22.396	-0.906
5500	8.936	85.686	77.327	45.975	-54.611	23.818	-0.946
5600	8.936	85.847	77.478	46.869	-54.895	25.250	-0.985
5700	8.936	86.006	77.626	47.762	-55.195	26.687	-1.023
5800	8.936	86.161	77.772	48.656	-55.512	28.126	-1.060
5900	8.937	86.314	77.916	49.550	-55.850	29.571	-1.095
6000	8.937	86.464	78.057	50.443	-56.213	31.030	-1.130

PLATINUM MONOXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

S^{o}_{298} = 60.495 e.u./gfw

$H^{o}_{298} - H^{o}_{0}$ = 2125 cal/gfw

ΔH^{o}_{f298} = 88.600 ± 15.000 Kcal/gfw

gfw = 211.09

Assumed and/or estimated molecular properties:

ω_e = 785 cm^{-1}

Pt-O bond distance = 1.85Å

B_e = 0.334 cm^{-1}

g = 6

TABLE VI - 12

RHENIUM OXIDE IDEAL MOLECULAR GAS ORe

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Re from 0° to 3453°K, Liquid Re from 3453° to 5960°K, Gaseous Re from 5960° to 6000°K; Gaseous O_2, Gaseous ReO.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-2.113	90.231	90.231	Infinite
298.15	7.515	59.382	59.382	0.000	90.000	82.250	-60.288
300	7.523	59.429	59.382	0.014	89.996	82.202	-59.881
400	7.905	61.647	59.682	0.786	89.791	79.636	-43.509
500	8.180	63.443	60.260	1.591	89.600	77.119	-33.707
600	8.368	64.952	60.920	2.419	89.408	74.640	-27.186
700	8.499	66.252	61.591	3.263	89.212	72.195	-22.539
800	8.591	67.393	62.246	4.118	89.004	69.778	-19.062
900	8.658	68.409	62.876	4.980	88.782	67.387	-16.363
1000	8.708	69.324	63.476	5.849	88.550	65.023	-14.210
1100	8.747	70.156	64.046	6.722	88.304	62.682	-12.453
1200	8.776	70.919	64.587	7.598	88.043	60.364	-10.993
1300	8.800	71.622	65.102	8.477	87.768	58.067	-9.762
1400	8.819	72.275	65.591	9.358	87.479	55.795	-8.710
1500	8.834	72.884	66.057	10.240	87.173	53.542	-7.801
1600	8.847	73.455	66.502	11.124	86.852	51.310	-7.008
1700	8.858	73.991	66.927	12.010	86.515	49.098	-6.312
1800	8.867	74.498	67.333	12.896	86.161	46.909	-5.695
1900	8.874	74.977	67.723	13.783	85.790	44.739	-5.146
2000	8.881	75.433	68.097	14.671	85.402	42.588	-4.654
2100	8.886	75.866	68.457	15.559	84.994	40.458	-4.210
2200	8.891	76.280	68.803	16.448	84.570	38.347	-3.809
2300	8.896	76.675	69.137	17.337	84.125	36.255	-3.445
2400	8.899	77.054	69.459	18.227	83.663	34.184	-3.113
2500	8.903	77.417	69.770	19.117	83.180	32.131	-2.809
2600	8.906	77.766	70.071	20.008	82.678	30.100	-2.530
2700	8.908	78.102	70.362	20.898	82.154	28.088	-2.273
2800	8.911	78.426	70.645	21.789	81.611	26.093	-2.037
2900	8.913	78.739	70.918	22.680	81.046	24.122	-1.818
3000	8.915	79.041	71.184	23.572	80.462	22.168	-1.615
3100	8.917	79.334	71.442	24.463	79.853	20.239	-1.427
3200	8.918	79.617	71.693	25.355	79.224	18.325	-1.251
3300	8.920	79.891	71.938	26.247	78.575	16.430	-1.088
3400	8.921	80.158	72.175	27.139	77.901	14.559	-0.936
3453	8.922	80.296	72.299	27.612	77.535	13.575	-0.859
3453	8.922	80.296	72.299	27.612	69.592	13.575	-0.859
3500	8.922	80.416	72.407	28.031	69.266	12.813	-0.800
3600	8.923	80.668	72.633	28.924	68.570	11.209	-0.680
3700	8.924	80.912	72.854	29.816	67.871	9.625	-0.568
3800	8.925	81.150	73.069	30.708	67.171	8.063	-0.464
3900	8.926	81.382	73.279	31.601	66.469	6.515	-0.365
4000	8.927	81.608	73.484	32.494	65.766	4.990	-0.273
4100	8.928	81.828	73.685	33.386	65.060	3.478	-0.185
4200	8.928	82.043	73.882	34.279	64.353	1.985	-0.103
4300	8.929	82.254	74.074	35.172	63.645	0.508	-0.026
4400	8.930	82.459	74.262	36.065	62.934	-0.952	0.047
4500	8.930	82.660	74.447	36.958	62.221	-2.399	0.116
4600	8.931	82.856	74.627	37.851	61.506	-3.822	0.182
4700	8.931	83.048	74.804	38.744	60.789	-5.231	0.243
4800	8.932	83.236	74.978	39.637	60.068	-6.631	0.302
4900	8.932	83.420	75.149	40.530	59.345	-8.012	0.357
5000	8.933	83.601	75.316	41.424	58.618	-9.380	0.410
5100	8.933	83.777	75.480	42.317	57.886	-10.730	0.460
5200	8.933	83.951	75.641	43.210	57.149	-12.066	0.507
5300	8.934	84.121	75.800	44.104	56.407	-13.395	0.552
5400	8.934	84.288	75.955	44.997	55.656	-14.701	0.595
5500	8.934	84.452	76.108	45.890	54.896	-15.993	0.635
5600	8.935	84.613	76.259	46.784	54.127	-17.276	0.674
5700	8.935	84.771	76.407	47.677	53.344	-18.545	0.711
5800	8.935	84.927	76.552	48.571	52.546	-19.791	0.746
5900	8.935	85.079	76.695	49.464	51.728	-21.026	0.779
5960.67	8.936	85.169	76.780	50.000	51.219	-21.762	0.798
5960.67	8.936	85.169	76.780	50.000	-117.096	-21.762	0.798
6000	8.936	85.229	76.836	50.358	-117.511	-21.132	0.770

RHENIUM OXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

S^{o}_{298} = 59.382 e.u./gfw

$H^{o}_{298} - H^{o}_{0}$ = 2113 cal/gfw

ΔH^{o}_{f298} = 90.000 ± 15.000 Kcal/gfw

gfw = 202.22

Assumed and/or estimated molecular properties:

ω_e = 858 cm^{-1}

Re - O bond distance = 1.80 Å

B_e = 0.355 cm^{-1}

g = 4

TABLE VI - 13

RHODIUM MONOXIDE IDEAL MOLECULAR GAS ORh

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Rh from 0° to 2239°K, Liquid Rh from 2239° to 3996°K, Gaseous Rh from 3996° to 6000°K; Gaseous O_2; Gaseous RhO.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-2.119	88.691	88.691	Infinite
298.15	7.575	57.727	57.727	0.000	88.400	80.739	-59.181
300	7.583	57.774	57.727	0.014	88.396	80.692	-58.781
400	7.965	60.011	58.030	0.792	88.209	78.152	-42.698
500	8.231	61.819	58.613	1.603	88.015	75.659	-33.069
600	8.411	63.336	59.277	2.436	87.806	73.208	-26.665
700	8.533	64.643	59.952	3.283	87.578	70.793	-22.101
800	8.619	65.788	60.612	4.141	87.330	68.412	-18.688
900	8.682	66.807	61.244	5.006	87.060	66.063	-16.042
1000	8.728	67.724	61.847	5.877	86.768	63.745	-13.931
1100	8.763	68.558	62.420	6.752	86.453	61.458	-12.210
1200	8.790	69.322	62.964	7.629	86.116	59.201	-10.781
1300	8.812	70.026	63.480	8.509	85.756	56.972	-9.577
1400	8.829	70.680	63.971	9.392	85.376	54.772	-8.550
1500	8.844	71.289	64.439	10.275	84.972	52.600	-7.663
1600	8.855	71.861	64.885	11.160	84.547	50.455	-6.892
1700	8.865	72.398	65.312	12.046	84.099	48.338	-6.214
1800	8.873	72.905	65.720	12.933	83.628	46.247	-5.615
1900	8.880	73.385	66.110	13.821	83.136	44.186	-5.082
2000	8.886	73.840	66.486	14.709	82.621	42.148	-4.605
2100	8.891	74.274	66.846	15.598	82.083	40.139	-4.177
2200	8.896	74.688	67.193	16.487	81.523	38.155	-3.790
2239	8.898	74.843	67.324	16.834	81.299	37.389	-3.649
2239	8.898	74.843	67.324	16.834	76.149	37.389	-3.649
2300	8.900	75.083	67.528	17.377	75.803	36.334	-3.452
2400	8.903	75.462	67.851	18.267	75.231	34.629	-3.153
2500	8.906	75.826	68.162	19.158	74.659	32.951	-2.880
2600	8.909	76.175	68.464	20.049	74.083	31.295	-2.630
2700	8.911	76.511	68.756	20.940	73.506	29.657	-2.400
2800	8.914	76.835	69.039	21.831	72.925	28.046	-2.189
2900	8.916	77.148	69.313	22.722	72.342	26.455	-1.994
3000	8.917	77.450	69.579	23.614	71.758	24.882	-1.813
3100	8.919	77.743	69.838	24.506	71.172	23.329	-1.645
3200	8.920	78.026	70.089	25.398	70.583	21.797	-1.489
3300	8.922	78.301	70.334	26.290	69.993	20.278	-1.343
3400	8.923	78.567	70.572	27.182	69.399	18.783	-1.207
3500	8.924	78.826	70.804	28.074	68.805	17.303	-1.080
3600	8.925	79.077	71.031	28.967	68.208	15.840	-0.962
3700	8.926	79.322	71.251	29.859	67.610	14.396	-0.850
3800	8.927	79.560	71.467	30.752	67.010	12.964	-0.746
3900	8.928	79.791	71.677	31.645	66.409	11.552	-0.647
3995.89	8.928	80.008	71.875	32.502	65.826	10.206	-0.558
3995.89	8.928	80.008	71.875	32.502	-52.319	10.206	-0.558
4000	8.928	80.017	71.883	32.538	-52.327	10.258	-0.560
4100	8.929	80.238	72.084	33.430	-52.610	11.824	-0.630
4200	8.930	80.453	72.281	34.323	-52.895	13.405	-0.697
4300	8.930	80.663	72.473	35.216	-53.184	14.990	-0.762
4400	8.931	80.869	72.662	36.109	-53.477	16.574	-0.823
4500	8.931	81.069	72.846	37.003	-53.771	18.173	-0.883
4600	8.932	81.266	73.027	37.896	-54.071	19.777	-0.940
4700	8.932	81.458	73.205	38.789	-54.375	21.378	-0.994
4800	8.933	81.646	73.379	39.682	-54.683	22.998	-1.047
4900	8.933	81.830	73.549	40.575	-54.995	24.624	-1.098
5000	8.933	82.010	73.717	41.469	-55.313	26.250	-1.147
5100	8.934	82.187	73.881	42.362	-55.638	27.883	-1.195
5200	8.934	82.361	74.042	43.256	-55.969	29.531	-1.241
5300	8.935	82.531	74.201	44.149	-56.309	31.179	-1.286
5400	8.935	82.698	74.357	45.042	-56.658	32.829	-1.329
5500	8.935	82.862	74.510	45.936	-57.016	34.497	-1.371
5600	8.935	83.023	74.661	46.829	-57.390	36.155	-1.411
5700	8.936	83.181	74.809	47.723	-57.776	37.835	-1.451
5800	8.936	83.337	74.954	48.617	-58.180	39.520	-1.489
5900	8.936	83.489	75.098	49.510	-58.605	41.212	-1.527
6000	8.936	83.639	75.239	50.404	-59.054	42.908	-1.563

RHODIUM MONOXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

S^{o}_{298} = 57.727 e.u./gfw

$H^{o}_{298} - H^{o}_{0}$ = 2119 cal/gfw

ΔH^{o}_{f298} = 88.400 ± 15.000 Kcal/gfw

gfw = 118.91

Assumed and/or estimated molecular properties:

ω_e = 820 cm^{-1}

Rh-O bond distance = 1.81 Å

B_e = 0.373 cm^{-1}

g = 4

TABLE VI - 14

STRONTIUM OXIDE CONDENSED PHASES OSr

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid Sr from 0° to 1045°K Liquid Sr from 1045° to 1641°K Gaseous Sr from 1641° to 4000°K Gaseous O_2 Solid SrO from 0° to 2690°K, Liquid SrO from 2690° to 4000°K

	cal/°K gfw			Kcal/gfw			
T °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0 000	0 000	Infinite	-2 038	-140 551	-140 551	Infinite
298 15	10 760	13 060	13 060	0 000	-141 100	-133 961	98 192
300	10 784	13 127	13 060	0 020	-141 099	-133 917	97 554
400	11 663	16 365	13 496	1 148	-140 987	131 539	71 866
500	12 138	19 023	14 343	2 340	-140 860	129 192	56 467
600	12 453	21 265	15 315	3 570	-140 749	126 868	46 210
700	12 694	23 204	16 307	4 828	-140 661	-124 563	38 888
800	12 894	24 912	17 278	6 108	-140 600	122 267	33 400
862	13 006	25 879	17 862	6 910	-140 578	-120 847	30 638
862	13 006	25 879	17 862	6 910	-140 778	-120 847	30 638
900	13 071	26 441	18 212	7 406	-140 786	119 969	29 131
1000	13 233	27 827	19 106	8 721	-140 800	-117 655	25 712
1045	13 303	28.411	19.494	9 318	-140 804	-116 613	24 387
1045	13 303	28 411	19 494	9 318	-142 774	116 613	24 387
1100	13 386	29 095	19 957	10 052	-142 701	-115 238	22 895
1200	13 532	30 266	20 768	11 398	-142 559	112 748	20 533
1300	13 674	31 355	21 541	12 758	-142 407	110 270	18 537
1400	13 813	32 374	22 279	14 133	-142 245	107 805	16 828
1500	13 949	33 331	22 984	15 521	-142 072	-105 350	15 349
1600	14 083	34 236	23 659	16 923	141 888	102 907	14 056
1640 43	14 138	34 593	23 928	17 501	-141 802	101 909	13 572
1640 43	14 138	34 593	23 928	17 501	-174 814	101 909	13 572
1700	14 216	35 094	24 307	18 338	174 531	99 288	12 764
1800	14 348	35 910	24 929	19 766	-174 046	-94 877	11 519
1900	14 479	36 689	25 527	21 207	-173 552	90 492	10 408
2000	14 609	37 435	26 104	22 662	-173 049	-86 133	9 412
2100	14 739	38 151	26 661	24 129	-172 539	-81 801	8 513
2200	14 868	38 840	27 199	25 609	-172 023	77 490	7 698
2300	14 997	39 503	27 720	27 103	-171 502	-73 204	6 956
2400	15 125	40 144	28 224	28 609	-170 978	-68 943	6 278
2500	15 253	40 764	28 713	30 128	-170 452	-64 705	5 656
2600	15 381	41.365	29 189	31 659	-169 926	-60 482	5 084
2690	15 496	41 891	29 605	33 049	-169 456	-56 707	4 607
2690	17 000	47 876	29 605	49 149	-153 356	-56 707	4 607
2700	17 000	47 939	29 673	49 319	-153 289	56 344	4 561
2800	17 000	48 557	30 336	51 019	-152 628	-52 766	4 118
2900	17 000	49 154	30 975	52 719	-151 988	-49 211	3 708
3000	17 000	49 730	31 590	54 419	151 369	45 675	3 327
3100	17 000	50 287	32 184	56 119	-150 774	-42 160	2 972
3200	17 000	50 827	32 759	57 819	-150 207	-38 669	2 641
3300	17 000	51 350	33 314	59 519	-149 669	-35 190	2 330
3400	17 000	51 858	33 852	61 219	-149 163	-31 731	2 040
3500	17 000	52 350	34 374	62 919	-148 689	-28 282	1 766
3600	17 000	52 829	34 880	64 619	-148 250	24 850	1 508
3700	17 000	53 295	35 371	66 319	-147 847	-21 428	1 266
3800	17 000	53 749	35 849	68 019	147 488	18 012	1 036
3900	17 000	54 190	36 313	69 719	-147 157	-14 611	0 819
4000	17 000	54 621	36 766	71 419	-146 870	-11 217	0 613

STRONTIUM OXIDE CONDENSED PHASES

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± 200	± .200	± .200	± .000	± 2 000	± 2 210	± 1.620
1000	± .940	± .650	± .390	± .260	± 2.440	± 2.960	± .650
2000	± 1.780	± .940	± .600	± .680	± 3.730	± 4.250	± .460
2690	± 2.680	± 1.070	± .700	± 990	± 4.040	± 4.930	± .400
2690	± 1.000	± 1.590	± .700	± 2.390	± 5.440	± 4.930	± .400
4000	± 2.000	± 2.190	± 1.100	± 4.350	± 7.400	± 7.450	± .410

Summary of Basic Data

Solid has a face-centered cubic (NaCl type) structure.

m.p.	b.p.
$T_m = 2690^\circ \pm 50^\circ K$	Decomposes at 1 atm at 4500°K
$\Delta H_m = 16.100 \pm 1.400$ Kcal/gfw	
$\Delta S_m = 5.985 \pm 0.520$ e.u./gfw	

$S_{298}^\circ = 13.060 \pm 0.200$ e.u./gfw

$H_{298}^\circ - H_0^\circ = 2038$ cal/gfw

$\Delta H_{f298}^\circ = -141.100 \pm 2.000$ Kcal/gfw

gfw = 103.63

Heat capacity of solid in cal/°K gfw obtained from

$$H_T^\circ - H_{298}^\circ = 12.13T + 0.63 \times 10^{-3}T^2 + 1.55 \times 10^5/T - 4192$$

C_p°(liquid) = 17.000 cal/°K gfw

TABLE VI - 15

STRONTIUM OXIDE | IDEAL MOLECULAR GAS | OSr

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Sr from 0° to 1045°K, Liquid Sr from 1045° to 1641°K, Gaseous Sr from 1641° to 6000°K, Gaseous O_2; Gaseous SrO.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-2.161	-11.874	-11.875	Infinite
298.15	7.910	57.145	57.145	0.000	-12.300	-18.305	13.417
300	7.918	57.194	57.145	0.015	-12.303	-18.342	13.362
400	8.277	59.525	57.460	0.826	-12.509	-20.325	11.104
500	8.501	61.398	58.067	1.666	-12.734	-22.254	9.727
600	8.644	62.961	58.756	2.523	-12.996	-24.133	8.790
700	8.742	64.302	59.454	3.393	-13.295	-25.966	8.107
800	8.813	65.474	60.135	4.271	-13.637	-27.753	7.581
862	8.848	66.133	60.543	4.818	-13.870	-28.838	7.311
862	8.848	66.133	60.543	4.818	-14.070	-28.838	7.311
900	8.866	66.515	60.787	5.155	-14.236	-29.486	7.160
1000	8.909	67.452	61.408	6.044	-14.677	-31.157	6.809
1045	8.925	67.844	61.676	6.445	-14.878	-31.894	6.670
1045	8.925	67.844	61.676	6.445	-16.848	-31.894	6.670
1100	8.944	68.302	61.996	6.936	-17.017	-32.681	6.493
1200	8.973	69.082	62.555	7.832	-17.325	-34.093	6.209
1300	9.000	69.801	63.085	8.731	-17.634	-35.477	5.964
1400	9.024	70.469	63.589	9.632	-17.946	-36.839	5.751
1500	9.046	71.093	64.069	10.536	-18.257	-38.177	5.562
1600	9.068	71.677	64.526	11.442	-18.569	-39.494	5.394
1640.43	9.077	71.907	64.708	11.813	-18.690	-40.029	5.331
1640.43	9.077	71.907	64.708	11.813	-51.702	-40.029	5.331
1700	9.089	72.228	64.963	12.349	-51.720	-39.604	5.091
1800	9.111	72.748	65.382	13.259	-51.753	-38.892	4.722
1900	9.132	73.242	65.783	14.172	-51.787	-38.177	4.391
2000	9.155	73.711	66.168	15.086	-51.825	-37.460	4.093
2100	9.177	74.158	66.538	16.002	-51.866	-36.743	3.824
2200	9.201	74.586	66.895	16.921	-51.912	-36.022	3.578
2300	9.226	74.996	67.238	17.843	-51.962	-35.297	3.354
2400	9.252	75.390	67.570	18.767	-52.020	-34.573	3.148
2500	9.278	75.768	67.891	19.693	-52.087	-33.849	2.959
2600	9.305	76.133	68.201	20.622	-52.164	-33.116	2.784
2700	9.334	76.485	68.502	21.554	-52.254	-32.384	2.621
2800	9.363	76.826	68.794	22.489	-52.358	-31.648	2.470
2900	9.392	77.156	69.077	23.427	-52.480	-30.908	2.329
3000	9.423	77.475	69.353	24.367	-52.621	-30.163	2.197
3100	9.454	77.785	69.620	25.311	-52.782	-29.410	2.073
3200	9.486	78.087	69.881	26.258	-52.968	-28.660	1.957
3300	9.518	78.380	70.135	27.208	-53.180	-27.899	1.848
3400	9.551	78.666	70.383	28.162	-53.420	-27.136	1.744
3500	9.585	78.944	70.624	29.119	-53.689	-26.358	1.646
3600	9.619	79.216	70.860	30.079	-53.990	-25.579	1.553
3700	9.653	79.481	71.091	31.042	-54.324	-24.791	1.464
3800	9.688	79.740	71.316	32.009	-54.692	-23.987	1.379
3900	9.724	79.993	71.537	32.980	-55.096	-23.183	1.299
4000	9.760	80.241	71.753	33.954	-55.535	-22.366	1.222
4100	9.796	80.484	71.964	34.931	-56.012	-21.533	1.148
4200	9.833	80.722	72.171	35.912	-56.525	-20.692	1.077
4300	9.870	80.955	72.375	36.897	-57.074	-19.838	1.008
4400	9.908	81.184	72.574	37.886	-57.659	-18.975	0.942
4500	9.946	81.409	72.769	38.878	-58.280	-18.092	0.879
4600	9.985	81.630	72.962	39.875	-58.935	-17.204	0.817
4700	10.024	81.847	73.150	40.875	-59.627	-16.295	0.758
4800	10.063	82.060	73.336	41.879	-60.351	-15.379	0.700
4900	10.103	82.270	73.518	42.887	-61.108	-14.444	0.644
5000	10.144	82.477	73.697	43.899	-61.897	-13.490	0.590
5100	10.184	82.681	73.874	44.915	-62.718	-12.530	0.537
5200	10.226	82.881	74.048	45.935	-63.569	-11.556	0.486
5300	10.267	83.079	74.219	46.959	-64.450	-10.554	0.435
5400	10.310	83.274	74.387	47.987	-65.363	-9.541	0.386
5500	10.352	83.466	74.553	49.020	-66.302	-8.513	0.338
5600	10.395	83.656	74.717	50.056	-67.274	-7.470	0.292
5700	10.439	83.843	74.878	51.097	-68.275	-6.400	0.245
5800	10.482	84.028	75.038	52.143	-69.307	-5.331	0.201
5900	10.526	84.210	75.195	53.193	-70.372	-4.229	0.157
6000	10.571	84.391	75.350	54.247	-71.473	-3.114	0.113

STRONTIUM OXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

S^o_{298} = 57.145 e.u./gfw

$H^o_{298}-H^o_0$ = 2161 cal/gfw

ΔH^o_{f298} = -12.303 ± 10.000 Kcal/gfw

gfw = 103.63

Spectroscopic constants for the assumed ground electronic state $\left({}^3\Sigma\right)$, from Kovacs, I. and A. Budo, Ann. Phys. 12, 17 (1953), constants for the A' state from Almkvist, G. and A. Lagerqvist, Ark. Fys. 1, 477 (1949), constants for the B' state from Mahanti, P. C., Phys. Rev. 42, 609 (1932) and Lagerqvist, A., Ark. Fys. 8, 83 (1954), and constants for the C' state from Lagerqvist, A. and G. Almkvist, Ark. Fys. 8, 481 (1954). Multiplicity of lowest ${}^1\Sigma$ state taken as 3.

TABLE VI - 16

TECHNETIUM MONOXIDE IDEAL MOLECULAR GAS OTc

Reference State for Calculating ΔH_f° ΔF_f° and Log K_p Solid Tc from 0° to 2473°K
Liquid Tc from 2473° to 4840°K Gaseous Tc from 4840° to 6000°K Gaseous O_2 Gaseous TcO

	cal/°K gfw			Kcal/gfw			
T °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0 000	0 000	Infinite	2 114	89 004	89 004	Infinite
298 15	7 521	57 538	57 538	0 000	88 600	81 136	-59 471
300	7 529	57 584	57 538	0 014	88 597	81 090	59 071
400	7 911	59 805	57 838	0 787	88 425	78 614	42 950
500	8 185	61 602	58 417	1 592	88 253	76 181	-33 297
600	8 373	63 112	59 077	2 421	88 074	73 783	-26 874
700	8 502	64 413	59 748	3 265	87 880	71 416	-22 296
800	8 594	65 554	60 404	4 120	87 664	69 079	-18 871
900	8 661	66 571	61 034	4 983	87 431	66 769	16 213
1000	8 710	67 486	61 634	5 852	87 175	64 488	-14 093
1100	8 748	68 318	62 204	6 725	86 898	62 232	-12 364
1200	8 778	69 080	62 746	7 601	86 600	60 002	-10 927
1300	8 801	69 784	63 261	8 480	86 280	57 798	-9 716
1400	8 820	70 437	63 750	9 361	85 939	55 620	8 682
1500	8 835	71 046	64 217	10 244	85 576	53 466	-7 790
1600	8 848	71 617	64 662	11 128	85 191	51 338	7 012
1700	8 858	72 153	65 087	12 013	84 784	49 235	-6 329
1800	8 867	72 660	65 493	12 900	84 356	47 158	-5 725
1900	8 875	73 140	65 883	13 787	83 906	45 102	-5 188
2000	8 881	73 595	66 258	14 675	83 433	43 072	-4 706
2100	8 887	74 028	66 617	15 563	82 938	41 068	-4 274
2200	8 892	74 442	66 964	16 452	82 422	39 084	-3 882
2300	8 896	74 837	67 298	17 341	81 881	37 125	-3 527
2400	8 900	75 216	67 620	18 231	81 320	35 192	-3 204
2473	8 902	75 483	67 848	18 881	80 896	33 796	-2 987
2473	8 902	75 483	67 848	18 881	75 208	33 796	-2 987
2500	8 903	75 579	67 931	19 121	75 053	33 344	-2 915
2600	8 906	75 929	68 232	20 012	74 478	31 687	-2 663
2700	8 909	76 265	68 523	20 903	73 900	30 052	-2 432
2800	8 911	76 589	68 805	21 794	73 320	28 439	-2 220
2900	8 913	76 902	69 079	22 685	72 737	26 846	-2 023
3000	8 915	77 204	69 345	23 576	72 152	25 275	-1 841
3100	8 917	77 496	69 603	24 468	71 565	23 722	-1 672
3200	8 918	77 779	69 854	25 360	70 976	22 189	-1 515
3300	8 920	78 054	70 099	26 251	70 385	20 670	1 369
3400	8 921	78 320	70 337	27 144	69 793	19 174	-1 232
3500	8 922	78 579	70 568	28 036	69 198	17 699	-1 105
3600	8 923	78 830	70 794	28 928	68 601	16 235	-0 986
3700	8 925	79 074	71 015	29 820	68 002	14 785	-0 873
3800	8 925	79 312	71 230	30 713	67 403	13 358	-0 768
3900	8 926	79 544	71 440	31 605	66 800	11 944	0 669
4000	8 927	79 770	71 646	32 498	66 197	10 542	-0 576
4100	8 928	79 991	71 847	33 391	65 592	9 158	-0 488
4200	8 929	80 206	72 043	34 284	64 985	7 792	-0 405
4300	8 929	80 416	72 235	35 177	64 377	6 440	0 327
4400	8 930	80 621	72 424	36 070	63 766	5 097	-0 253
4500	8 930	80 822	72 608	36 963	63 153	3 770	-0 183
4600	8 931	81 018	72 789	37 856	62 538	2 456	-0 117
4700	8 931	81 210	72 966	38 749	61 921	1 161	-0 054
4800	8 932	81 398	73 140	39 642	61 300	-0 126	0 006
4840 07	8 932	81 472	73 208	39 999	61 050	-0 640	0 029
4840 07	8 932	81 472	73 208	39 999	-78 822	-0 640	0 029
4900	8 932	81 583	73 310	40 535	-79 045	0 339	-0 015
5000	8 933	81 763	73 477	41 428	79 426	1 960	-0 086
5100	8 933	81 940	73 642	42 322	-79 815	3 588	-0 154
5200	8 933	82 113	73 803	43 215	-80 213	5 234	-0 220
5300	8 934	82 284	73 961	44 108	-80 621	6 877	-0 284
5400	8 934	82 451	74 117	45 002	-81 039	8 534	-0 345
5500	8 934	82.614	74 270	45 895	-81 469	10 200	-0 405
5600	8 935	82 775	74 420	46 789	-81 912	11 877	-0 464
5700	8 935	82 934	74 568	47 682	-82 371	13 554	-0 520
5800	8 935	83 089	74 714	48 576	-82 848	15 239	-0 574
5900	8 936	83.242	74 857	49 469	-83 346	16 939	-0 627
6000	8 936	83 392	74 998	50 363	-83 868	18 646	-0 679

TECHNETIUM MONOXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

S^{o}_{298} = 57.538 e.u./gfw

$H^{o}_{298} - H^{o}_{0}$ = 2114 cal/gfw

ΔH^{o}_{f298} = 88.600 ± 15.000 Kcal/gfw

gfw = 115*

Assumed and/or estimated molecular properties·

ω_e = 854 cm^{-1}

Tc-O bond distance = 1.78Å

B_e = 0.385 cm^{-1}

g = 4

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* Using Tc isotope of longest known half-life

TABLE VI - 17

THORIUM MONOXIDE IDEAL MOLECULAR GAS OTh

Reference State for Calculating ΔH_f^o ΔF_f^o and Log K_p Solid Th from 0° to 2028°K
Liquid Th from 2028° to 5060°K Gaseous Th from 5060° to 6000°K Gaseous O_2 Gaseous ThO

	cal °K gfw			Kcal gfw			
T °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
0	0 000	0 000	Infinite	-2 125	7 172	-7 172	Infinite
298 15	7 627	58 836	58 836	0 000	-7 640	14 399	10 554
300	7 636	58 883	58 836	0 014	7 649	-14 441	10 520
400	8 033	61 137	59 141	0 798	-8 084	16 639	9 091
500	8 340	62 963	59 728	1 618	8 493	-18 730	8 186
600	8 602	64 508	60 399	2 465	8 888	20 739	7 554
700	8 851	65 852	61 084	3 338	-9 268	-22 684	7 082
800	9 095	67 050	61 756	4 235	-9 634	24 576	6 713
900	9 331	68 135	62 406	5 156	-9 984	26 423	6 416
1000	9 551	69 130	63 029	6 101	-10 317	28 231	6 169
1100	9 750	70 050	63 626	7 066	-10 635	30 007	5 962
1200	9 923	70 906	64 198	8 050	10 939	-31 755	5 783
1300	10 067	71 706	64 745	9 050	-11 232	-33 478	5 628
1400	10 183	72 456	65 269	10 062	-11 516	-35 178	5 491
1500	10 273	73 162	65 772	11 085	11 792	-36 859	5 370
1600	10 338	73 827	66 255	12 116	-12 063	-38 521	5 261
1633	10 354	74 039	66 410	12 457	-12 152	39 066	5 228
1633	10 354	74 039	66 410	12 457	-12 806	-39 066	5 228
1700	10 382	74 456	66 719	13 152	-13 144	-40 137	5 160
1800	10 408	75 050	67 166	14 192	13 648	-41 711	5 064
1900	10 419	75 613	67 595	15 233	-14 154	43 255	4 975
2000	10 418	76 147	68 010	16 275	-14 662	44 774	4 892
2028	10 417	76 292	68 123	16 567	-14 805	-45 195	4 870
2028	10 417	76 292	68 123	16 567	-18 658	-45 195	4 870
2100	10 408	76 656	68 410	17 317	-19 026	-46 130	4 801
2200	10 391	77 140	68 796	18 357	-19 542	-47 408	4 709
2300	10 368	77 601	69 169	19 395	-20 062	-48 664	4 624
2400	10 342	78 042	69 529	20 430	-20 588	-49 896	4 543
2500	10 312	78 464	69 879	21 463	-21 119	-51 109	4 468
2600	10 281	78 868	70 217	22 493	-21 655	-52 296	4 396
2700	10 249	79 255	70 544	23 519	-22 197	-53 466	4 328
2800	10 217	79 628	70 862	24 542	-22 745	-54 613	4 263
2900	10 186	79 986	71 171	25 563	-23 299	-55 744	4 201
3000	10 154	80 331	71 471	26 580	-23 858	-56 854	4 142
3100	10 124	80 664	71 762	27 594	-24 422	-57 942	4 085
3200	10 095	80 985	72 046	28 604	24 993	-59 018	4 031
3300	10 067	81 295	72 322	29 613	-25 567	-60 074	3 978
3400	10 040	81 596	72 590	30 618	26 146	-61 107	3 928
3500	10 015	81 887	72 852	31 621	-26 731	62 130	3 879
3600	9 991	82 169	73 107	32 621	-27 320	-63 132	3 832
3700	9 969	82 443	73 356	33 619	-27 912	64 121	3 787
3800	9 948	82 709	73 599	34 615	-28 509	-65 094	3 744
3900	9 928	82 967	73 837	35 609	29 109	-66 052	3 701
4000	9 910	83 219	74 069	36 600	-29 714	-66 994	3 660
4100	9 893	83 464	74 295	37 591	-30 321	67 918	3 620
4200	9 877	83 702	74 517	38 579	-30 933	-68 830	3 581
4300	9 862	83 935	74 734	39 566	-31 548	-69 728	3 544
4400	9 849	84 162	74 956	40 552	-32 166	-70 652	3 509
4500	9 836	84 384	75 154	41 536	-32 787	-71 477	3 471
4600	9 825	84 601	75 357	42 519	33 412	-72 330	3 436
4700	9 815	84 813	75 557	43 501	-34 041	73 177	3 403
4800	9 805	85 020	75 753	44 482	-34 673	74 002	3 369
4900	9 797	85 223	75 945	45 462	35 309	-74 817	3 337
5000	9 790	85 421	76 133	46 441	-35 951	-75 620	3 305
5060 26	9 785	85 538	76 244	47 0[illegible]	-36 341	-76 092	3 286
5060 26	9 785	85 538	76 244	47 [illegible]9	159 106	-76 092	3 286
5100	9 783	85 616	76 318	47 [illegible]0	-159 296	-75 450	3 233
5200	9 777	85 806	76 499	48 398	-159 785	-73 805	3 102
5300	9 772	85 993	76 677	49 375	-160 286	72 144	2 975
5400	9 767	86 177	76 852	50 352	-160 798	-70 480	2 852
5500	9 763	86 357	77 025	51 329	161 321	-68 814	2 734
5600	9 760	86 534	77 194	52 305	-161 860	-67 126	2 620
5700	9 758	86 708	77 360	53 281	162 414	-65 432	2 509
5800	9 756	86 878	77 524	54 257	-162 986	-63 729	2 401
5900	9 755	87 046	77 685	55 232	163 580	-62 014	2 297
6000	9 754	87 211	77 843	56 207	-164 198	-60 290	2 196

THORIUM MONOXIDE IDEAL MOLECULAR GAS

Summary of Basic Data

S^{o}_{298} = 58.836 e.u /gfw

$H^{o}_{298}-H^{o}_{0}$ = 2125 cal/gfw

ΔH^{o}_{f298} = -7.640 Kcal/gfw

gfw = 248.05

Spectroscopic constants derived from data of Krishnamurty, S. G., Proc. Phys. Soc. (London) 64A, 852 (1951). Assumed and/or estimated molecular properties in units of cm^{-1} for $X^{3}\pi$ electronic state:

E	ω_e	$\omega_e x_e$	B_e	α_e	D_e
0, 2721, 4177	800	3.5	0.327	0.0018	2.2×10^{-7}

TABLE VI - 18

PLATINUM | REFERENCE STATE | Pt

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid from 0° to 2043°K,
Liquid from 2043° to 4108°K, Gas from 4108° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-1.372			
298.15	6.180	9.950	9.950	0.000			
300	6.183	9.988	9.950	0.011			
400	6.339	11.790	10.195	0.638			
500	6.464	13.218	10.661	1.278			
600	6.583	14.407	11.189	1.931			
700	6.704	15.431	11.724	2.595			
800	6.827	16.334	12.245	3.272			
900	6.951	17.145	12.745	3.960			
1000	7.076	17.884	13.222	4.662			
1100	7.201	18.564	13.677	5.376			
1200	7.326	19.196	14.111	6.102			
1300	7.452	19.788	14.525	6.841			
1400	7.577	20.344	14.921	7.592			
1500	7.703	20.871	15.301	8.356			
1600	7.828	21.373	15.665	9.133			
1700	7.954	21.851	16.014	9.922			
1800	8.080	22.309	16.352	10.724			
1900	8.206	22.749	16.677	11.538			
2000	8.332	23.174	16.991	12.365			
2043	8.386	23.351	17.149	12.724			
2043	8.500	25.651	17.149	17.423			
2100	8.500	25.885	17.358	17.908			
2200	8.500	26.281	17.754	18.758			
2300	8.500	26.659	18.133	19.608			
2400	8.500	27.020	18.496	20.458			
2500	8.500	27.367	18.844	21.308			
2600	8.500	27.701	19.178	22.158			
2700	8.500	28.021	19.500	23.008			
2800	8.500	28.331	19.810	23.858			
2900	8.500	28.629	20.109	24.708			
3000	8.500	28.917	20.398	25.558			
3100	8.500	29.196	20.677	26.408			
3200	8.500	29.466	20.948	27.258			
3300	8.500	29.727	21.210	28.108			
3400	8.500	29.981	21.464	28.958			
3500	8.500	30.227	21.711	29.808			
3600	8.500	30.467	21.951	30.658			
3700	8.500	30.700	22.184	31.508			
3800	8.500	30.926	22.411	32.358			
3900	8.500	31.147	22.632	33.208			
4000	8.500	31.362	22.848	34.058			
4100	8.500	31.572	23.058	34.908			
4108.34	8.500	31.589	23.126	34.979			
4108.34	5.829	61.168	23.126	156.498			
4200	5.850	61.297	23.908	157.032			
4300	5.873	61.435	24.779	157.619			
4400	5.895	61.570	25.614	158.207			
4500	5.917	61.703	26.415	158.798			
4600	5.939	61.833	27.183	159.390			
4700	5.960	61.961	27.922	159.985			
4800	5.982	62.087	28.632	160.583			
4900	6.003	62.210	29.316	161.182			
5000	6.024	62.332	29.975	161.783			
5100	6.046	62.451	30.610	162.387			
5200	6.067	62.569	31.224	162.992			
5300	6.089	62.685	31.817	163.600			
5400	6.111	62.799	32.390	164.210			
5500	6.133	62.911	32.943	164.822			
5600	6.155	63.022	33.480	165.437			
5700	6.178	63.131	33.999	166.053			
5800	6.202	63.239	34.502	166.672			
5900	6.225	63.345	34.990	167.294			
6000	6.250	63.450	35.464	167.917			

PLATINUM REFERENCE STATE

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
298.15	± .020	± .050	± .050	± .000			
1000	± .020	± .070	± .060	± .010			
2043	± .100	± .120	± .080	± .080			
2043	± .420	± .510	± .080	± .880			
3000	± 2.050	± .980	± .290	± 2.060			
4000	± 3.750	± 1.810	± .570	± 4.960			
4108.34	± 3.930	± 1.910	± .610	± 5.370			
4108.34	± .000	± .003	± .003	± .001			
5000	± .001	± .003	± .003	± .001			
6000	± .001	± .003	± .003	± .002			

Summary of Basic Data

Solid has face-centered cubic (A1 type) of structure.

m.p. = 2043° ± 3°K

ΔH_m = 4699 ± 800 cal/gfw

ΔS_m = 2.300 ± .390 e.u./gfw

b.p. = 4108° ± 95°K

ΔH_m = 121.519 ± 5.670 Kcal/gfw

ΔS_m = 29.579 ± 1.453 e.u./gfw

S_{298}^o = 9.950 ± .050 e.u./gfw $H_{298}^o - H_0^o$ = 1372 cal/gfw gfw = 195.09

C_p^o(298° to 500°K) $= 6.028 + 0.969 \times 10^{-3}T - 0.1220 \times 10^{5}T^{-2}$ (cal/°K gfw)

C_p^o(500° to 2043°K) $= 5.810 + 1.260 \times 10^{-3}T - 0.060 \times 10^{5}T^{-2}$ (cal/°K gfw)

C_p^o(liquid) = 8.500 cal/°K gfw

TABLE VI - 19

PLATINUM IDEAL MONATOMIC GAS **Pt**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid from 0° to 2043°K, Liquid from 2043° to 4108°K, Gas from 4108° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-1.572	134.900	134.900	Infinite
298.15	6.102	45.962	45.962	0.000	135.100	124.363	-91.156
300	6.113	45.999	45.962	0.011	135.100	124.296	-90.545
400	6.459	47.817	46.207	0.644	135.106	120.695	-65.942
500	6.435	49.260	46.679	1.291	135.113	117.091	-51.178
600	6.260	50.419	47.209	1.926	135.095	113.488	-41.336
700	6.059	51.369	47.738	2.542	135.047	109.890	-34.308
800	5.877	52.166	48.243	3.138	134.966	106.302	-29.039
900	5.728	52.849	48.717	3.718	134.858	102.725	-24.944
1000	5.609	53.446	49.161	4.285	134.723	99.161	-21.671
1100	5.517	53.976	49.575	4.841	134.565	95.612	-18.995
1200	5.447	54.453	49.962	5.389	134.387	92.079	-16.769
1300	5.395	54.887	50.325	5.931	134.190	88.560	-14.888
1400	5.358	55.285	50.665	6.469	133.977	85.058	-13.278
1500	5.333	55.654	50.985	7.003	133.747	81.574	-11.885
1600	5.318	55.998	51.288	7.536	133.503	78.103	-10.668
1700	5.311	56.320	51.575	8.067	133.245	74.646	-9.596
1800	5.310	56.623	51.847	8.598	132.974	71.209	-8.646
1900	5.316	56.911	52.106	9.129	132.691	67.785	-7.797
2000	5.326	57.184	52.353	9.661	132.396	64.376	-7.034
2043	5.332	57.294	52.453	9.891	132.267	62.921	-6.731
2043	5.332	57.294	52.453	9.891	127.568	62.921	-6.731
2100	5.340	57.444	52.589	10.195	127.387	61.115	-6.360
2200	5.356	57.693	52.816	10.729	127.071	57.964	-5.758
2300	5.376	57.931	53.033	11.266	126.758	54.830	-5.210
2400	5.397	58.160	53.242	11.805	126.447	51.710	-4.709
2500	5.421	58.381	53.443	12.346	126.138	48.602	-4.249
2600	5.445	58.594	53.637	12.889	125.831	45.507	-3.825
2700	5.470	58.800	53.824	13.435	125.527	42.425	-3.434
2800	5.496	59.000	54.006	13.983	125.225	39.351	-3.071
2900	5.523	59.193	54.181	14.534	124.926	36.291	-2.735
3000	5.549	59.381	54.351	15.087	124.629	33.241	-2.421
3100	5.576	59.563	54.517	15.644	124.336	30.196	-2.129
3200	5.603	59.740	54.677	16.203	124.045	27.167	-1.855
3300	5.629	59.913	54.833	16.764	123.756	24.144	-1.599
3400	5.655	60.082	54.985	17.328	123.470	21.129	-1.358
3500	5.681	60.246	55.133	17.895	123.187	18.123	-1.132
3600	5.707	60.406	55.277	18.465	122.907	15.126	-0.918
3700	5.732	60.563	55.418	19.037	122.629	12.134	-0.717
3800	5.756	60.716	55.555	19.611	122.353	9.153	-0.526
3900	5.780	60.866	55.690	20.188	122.080	6.174	-0.346
4000	5.804	61.013	55.821	20.767	121.809	3.208	-0.175
4100	5.827	61.156	55.949	21.349	121.541	0.247	-0.013
4108.34	5.829	61.168	55.960	21.398	121.519	0.000	0.000
4108.34	5.829	61.168	55.960	21.398			
4200	5.850	61.297	56.075	21.932			
4300	5.873	61.435	56.198	22.519			
4400	5.895	61.570	56.319	23.107			
4500	5.917	61.703	56.437	23.698			
4600	5.939	61.833	56.553	24.290			
4700	5.960	61.961	56.666	24.885			
4800	5.982	62.087	56.778	25.483			
4900	6.003	62.210	56.888	26.082			
5000	6.024	62.332	56.995	26.683			
5100	6.046	62.451	57.101	27.287			
5200	6.067	62.569	57.205	27.892			
5300	6.089	62.685	57.307	28.500			
5400	6.111	62.799	57.408	29.110			
5500	6.133	62.911	57.507	29.722			
5600	6.155	63.022	57.605	30.337			
5700	6.178	63.131	57.701	30.953			
5800	6.202	63.239	57.795	31.572			
5900	6.225	63.345	57.888	32.194			
6000	6.250	63.450	57.980	32.817			

PLATINUM IDEAL MONATOMIC GAS

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
298 15	± 000	± 002	± 003	± 000	± 300	± 320	± 230
1000	± 000	± 003	± 003	± 000	± 310	± 360	± 080
2000	± 000	± 003	± 003	± 000	—	—	—
2043	± 000	± 003	± 003	± 000	± 380	± 470	± 050
2043	± 000	± 003	± 003	± 000	± 1 180	± 470	± 050
3000	± 000	± 003	± 003	± 001	± 2 360	± 1 180	± 090
4000	± 000	± 003	± 003	± 001	± 5 260	± 2 590	± 140
4108 34	± 000	± 003	± 003	± 001	± 5 670	± 2 820	± 150
4108 34	± 000	± 003	± 003	± 001			
5000	± 001	± 003	± 003	± 001			
6000	± 001	± 003	± 003	± 002			

Summary of Basic Data

S_{298}^o = 45 962 ± .002 e u /gfw

$H_{298}^o - H_0^o$ = 1572 cal/gfw

ΔH_{f298}^o - 135 100 ± 300 Kcal/gfw

gfw = 195 09

Spectroscopic energy levels from Moore, C , Nat Bur Stds Circular 467, Vol. 3 (1 May 1958)

TABLE VI - 20

RHENIUM REFERENCE STATE Re

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid from 0° to 3453°K,
Liquid from 3453° to 5960°K, Gas from 5960° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
0	0.000	0.000	Infinite	-1.307			
298.15	6.160	8.886	8.886	0.000			
300	6.162	8.924	8.886	0.011			
400	6.262	10.710	9.129	0.633			
500	6.365	12.119	9.591	1.264			
600	6.472	13.289	10.112	1.906			
700	6.583	14.295	10.640	2.558			
800	6.697	15.181	11.153	3.222			
900	6.815	15.977	11.645	3.898			
1000	6.956	16.701	12.115	4.585			
1100	7.061	17.368	12.563	5.285			
1200	7.189	17.988	12.989	5.998			
1300	7.321	18.568	13.396	6.723			
1400	7.456	19.116	13.786	7.462			
1500	7.595	19.635	14.158	8.215			
1600	7.738	20.130	14.516	8.981			
1700	7.884	20.603	14.860	9.762			
1800	8.033	21.058	15.192	10.558			
1900	8.186	21.496	15.513	11.369			
2000	8.343	21.920	15.822	12.195			
2100	8.503	22.331	16.123	13.038			
2200	8.667	22.730	16.414	13.896			
2300	8.834	23.119	16.697	14.771			
2400	9.005	23.499	16.973	15.663			
2500	9.179	23.870	17.241	16.572			
2600	9.357	24.233	17.503	17.499			
2700	9.539	24.590	17.759	18.444			
2800	9.723	24.940	18.009	19.407			
2900	9.912	25.285	18.254	20.389			
3000	10.104	25.624	18.494	21.389			
3100	10.300	25.958	18.730	22.410			
3200	10.499	26.289	18.961	23.450			
3300	10.701	26.615	19.188	24.509			
3400	10.908	26.937	19.411	25.590			
3453	11.018	27.107	19.528	26.171			
3453	11.000	29.407	19.528	34.113			
3500	11.000	29.556	19.661	34.630			
3600	11.000	29.865	19.940	35.730			
3700	11.000	30.167	20.213	36.830			
3800	11.000	30.460	20.479	37.930			
3900	11.000	30.746	20.738	39.030			
4000	11.000	31.024	20.992	40.130			
4100	11.000	31.296	21.240	41.230			
4200	11.000	31.561	21.483	42.330			
4300	11.000	31.820	21.720	43.430			
4400	11.000	32.073	21.952	44.530			
4500	11.000	32.320	22.180	45.630			
4600	11.000	32.562	22.403	46.730			
4700	11.000	32.798	22.622	47.830			
4800	11.000	33.030	22.836	48.930			
4900	11.000	33.257	23.047	50.030			
5000	11.000	33.479	23.253	51.130			
5100	11.000	33.697	23.456	52.230			
5200	11.000	33.910	23.655	53.330			
5300	11.000	34.120	23.850	54.430			
5400	11.000	34.326	24.042	55.530			
5500	11.000	34.527	24.231	56.630			
5600	11.000	34.726	24.417	57.730			
5700	11.000	34.920	24.599	58.830			
5800	11.000	35.112	24.779	59.930			
5900	11.000	35.300	24.956	61.030			
5960.67	11.000	35.412	25.061	61.696			
5960.67	13.157	63.650	25.061	230.011			
6000	13.178	63.738	25.316	230.530			

RHENIUM REFERENCE STATE

Summary of Uncertainty Estimates

	cal/°K gfw				Kcal/gfw		
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± .040	± .050	± .050	± .000			
1000	± .100	± .090	± .070	± .020			
2000	± .500	± .290	± .130	± .320			
3000	± 1.000	± .600	± .240	± 1.070			
3453	± 1.500	± .770	± .300	± 1.640			
3453	± 1.550	± 1.210	± .300	± 3.140			
4000	± 1.750	± 1.380	± .440	± 3.770			
5000	± 3.950	± 2.010	± .690	± 6.620			
5960.67	± 6.070	± 2.890	± .970	± 11.430			
5960.67	± .009	± .005	± .003	± .012			

Summary of Basic Data

Solid has hexagonal close-packed (A3 type) structure.

m.p. = 3453° ±.20°K
ΔH_m = 7.942 ± 1.500 Kcal/gfw
ΔS_m = 2.300 ± .440 e.u./gfw

b.p. = 5960° ± 260°K
ΔH_v = 168.315 ± 12.940 Kcal/gfw
ΔS_v = 28.238 ± 3.560 e.u./gfw

S_{298}° = 8.886 ± .050 e.u./gfw $H_{298}^\circ - H_0^\circ$ = 1307 cal/gfw   gfw = 186.22

C_p°(solid) = $5.883 + 0.876 \times 10^{-3}T + 0.0177 \times 10^{-5}T^2$ (cal/°K gfw)

C_p°(liquid) = 11.000 cal/°K gfw

TABLE VI - 21

RHENIUM IDEAL MONATOMIC GAS Re

Reference State for Cálculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid from 0° to 3453°K,
Liquid from 3453° to 5960°K, Gas from 5960° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
0	0.000	0.000	Infinite	-1.481	185.196	185.196	Infinite
298.15	4.968	45.133	45.133	0.000	185.370	174.563	-127.952
300	4.968	45.163	45.133	0.009	185.368	174.496	-127.114
400	4.968	46.593	45.328	0.506	185.243	170.890	-93.366
500	4.968	47.701	45.696	1.003	185.109	167.318	-73.131
600	4.968	48.607	46.108	1.500	184.964	163.772	-59.651
700	4.968	49.373	46.521	1.996	184.808	160.253	-50.031
800	4.968	50.036	46.920	2.493	184.641	156.756	-42.822
900	4.968	50.622	47.299	2.990	184.462	153.281	-37.220
1000	4.968	51.145	47.658	3.487	184.272	149.827	-32.743
1100	4.968	51.619	47.997	3.984	184.069	146.393	-29.084
1200	4.969	52.051	48.317	4.481	183.853	142.976	-26.038
1300	4.971	52.449	48.620	4.978	183.634	139.579	-23.464
1400	4.974	52.817	48.907	5.475	183.383	136.201	-21.261
1500	4.979	53.160	49.179	5.972	183.127	132.838	-19.354
1600	4.989	53.482	49.438	6.471	182.860	129.495	-17.687
1700	5.004	53.785	49.685	6.970	182.578	126.168	-16.291
1800	5.025	54.071	49.921	7.472	182.284	122.858	-14.916
1900	5.056	54.344	50.146	7.976	181.977	119.567	-13.753
2000	5.097	54.604	50.363	8.483	181.658	116.288	-12.707
2100	5.150	54.854	50.571	8.995	181.327	113.029	-11.762
2200	5.218	55.095	50.771	9.514	180.988	109.785	-10.906
2300	5.301	55.329	50.964	10.040	180.639	106.556	-10.125
2400	5.401	55.557	51.151	10.574	180.281	103.343	-9.410
2500	5.518	55.779	51.331	11.120	179.918	100.145	-8.754
2600	5.655	55.998	51.507	11.679	179.550	96.960	-8.150
2700	5.810	56.215	51.677	12.252	179.178	93.791	-7.591
2800	5.984	56.429	51.843	12.841	178.804	90.635	-7.074
2900	6.178	56.642	52.005	13.449	178.430	87.492	-6.593
3000	6.390	56.855	52.163	14.078	178.059	84.363	-6.146
3100	6.620	57.069	52.318	14.728	177.688	81.247	-5.728
3200	6.866	57.283	52.469	15.402	177.322	78.144	-5.337
3300	7.127	57.498	52.619	16.101	176.962	75.048	-4.970
3400	7.402	57.715	52.765	16.828	176.608	71.966	-4.626
3453	7.552	57.830	52.842	17.224	176.423	70.337	-4.452
3453	7.552	57.830	52.842	17.224	168.481	70.337	-4.452
3500	7.688	57.933	52.910	17.582	168.322	68.998	-4.308
3600	7.984	58.154	53.052	18.366	168.006	66.167	-4.017
3700	8.288	58.377	53.193	19.179	167.719	63.344	-3.741
3800	8.596	58.602	53.333	20.023	167.463	60.525	-3.481
3900	8.908	58.829	53.471	20.899	167.239	57.711	-3.234
4000	9.220	59.059	53.608	21.805	167.045	54.906	-3.000
4100	9.531	59.290	53.743	22.743	166.883	52.108	-2.777
4200	9.838	59.524	53.878	23.711	166.751	49.311	-2.566
4300	10.138	59.759	54.012	24.710	166.650	46.514	-2.364
4400	10.431	59.995	54.145	25.739	166.579	43.721	-2.171
4500	10.714	60.233	54.278	26.796	166.536	40.929	-1.988
4600	10.986	60.471	54.410	27.881	166.521	38.138	-1.812
4700	11.244	60.710	54.542	28.993	166.533	35.346	-1.644
4800	11.489	60.950	54.673	30.129	166.569	32.552	-1.482
4900	11.719	61.189	54.803	31.290	166.630	29.766	-1.328
5000	11.932	61.428	54.933	32.473	166.713	26.970	-1.179
5100	12.130	61.666	55.063	33.676	166.816	24.174	-1.036
5200	12.311	61.903	55.192	34.898	166.938	21.378	-0.898
5300	12.475	62.139	55.321	36.138	167.078	18.574	-0.766
5400	12.623	62.374	55.450	37.393	167.233	15.767	-0.638
5500	12.754	62.607	55.578	38.662	167.402	12.962	-0.515
5600	12.869	62.838	55.705	39.943	167.583	10.157	-0.396
5700	12.968	63.066	55.832	41.235	167.775	7.342	-0.281
5800	13.052	63.293	55.959	42.536	167.976	4.526	-0.171
5900	13.122	63.516	56.085	43.845	168.185	1.709	-0.063
5960.67	13.157	63.650	56.161	44.641	168.315	0.000	0.000
5960.67	13.157	63.650	56.161	44.641			
6000	13.178	63.738	56.211	45.160			

RHENIUM IDEAL MONATOMIC GAS

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
298.15	± .000	± .002	± .002	± .000	± 1.500	± 1.520	± 1.110
1000	± .000	± .002	± .003	± .000	± 1.520	± 1.570	± .340
2000	± .000	± .002	± .003	± .000	± 1.820	± 1.760	± .192
3000	± .001	± .003	± .003	± .001	± 2.570	± 2.220	± .160
3453	± .002	± .003	± .003	± .001	± 3.140	± 2.540	± .160
3453	± .002	± .003	± .003	± .001	± 4.640	± 2.540	± .160
4000	± .003	± .003	± .003	± .002	± 5.270	± 3.260	± .180
5000	± 006	± .004	± .003	± .006	± 8.130	± 4.950	± .220
5960.67	± .009	± .005	± .003	± .012	± 12.940	± 7.280	± .270
5960.67	± .009	± .005	± .003	± .012	—	—	—

Summary of Basic Data

S_{298}^o = 45.133 ± .002 e.u./gfw

$H_{298}^o - H_0^o$ = 1481 cal/gfw

ΔH_{f298}^o = 185.370 ± 1.500 Kcal/gfw

gfw = 186.22

Spectroscopic energy levels from Moore, C., Nat. Bur. Stds. Circular 467, Vol. 3 (1958).

TABLE VI - 22

RHODIUM

REFERENCE STATE

Rh

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid from 0° to 2239°K, Liquid from 2239° to 3996°K, Gas from 3996° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-1.174			
298.15	5.940	7.530	7.530	0.000			
300	5.947	7.567	7.530	0.011			
400	6.262	9.323	7.768	0.622			
500	6.517	10.748	8.224	1.262			
600	6.747	11.957	8.749	1.925			
700	6.966	13.014	9.284	2.611			
800	7.180	13.958	9.810	3.318			
900	7.389	14.816	10.320	4.046			
1000	7.597	15.605	10.810	4.795			
1100	7.803	16.339	11.279	5.566			
1200	8.008	17.026	11.729	6.356			
1300	8.212	17.675	12.162	7.167			
1400	8.416	18.292	12.579	7.999			
1500	8.620	18.879	12.979	8.850			
1600	8.823	19.442	13.365	9.723			
1700	9.026	19.983	13.738	10.615			
1800	9.229	20.504	14.100	11.528			
1900	9.432	21.009	14.451	12.461			
2000	9.634	21.498	14.791	13.414			
2100	9.837	21.973	15.122	14.388			
2200	10.039	22.435	15.444	15.381			
2239	10.118	22.612	15.567	15.774			
2239	10.000	24.912	15.567	20.924			
2300	10.000	25.181	15.818	21.534			
2400	10.000	25.606	16.217	22.534			
2500	10.000	26.015	16.601	23.534			
2600	10.000	26.407	16.971	24.534			
2700	10.000	26.784	17.327	25.534			
2800	10.000	27.148	17.672	26.534			
2900	10.000	27.499	18.005	27.534			
3000	10.000	27.838	18.327	28.534			
3100	10.000	28.166	18.639	29.534			
3200	10.000	28.483	18.941	30.534			
3300	10.000	28.791	19.235	31.534			
3400	10.000	29.090	19.521	32.534			
3500	10.000	29.379	19.798	33.534			
3600	10.000	29.661	20.068	34.534			
3700	10.000	29.935	20.331	35.534			
3800	10.000	30.202	20.588	36.534			
3900	10.000	30.461	20.837	37.534			
3995.89	10.000	30.706	21.072	38.497			
3995.89	6.763	60.269	21.072	156.642			
4000	6.764	60.275	21.108	156.667			
4100	6.778	60.442	22.065	157.344			
4200	6.793	60.606	22.982	158.022			
4300	6.808	60.766	23.859	158.702			
4400	6.823	60.923	24.699	159.384			
4500	6.839	61.076	25.506	160.067			
4600	6.854	61.227	26.281	160.752			
4700	6.870	61.374	27.025	161.438			
4800	6.887	61.519	27.743	162.126			
4900	6.903	61.661	28.434	162.815			
5000	6.920	61.801	29.100	163.506			
5100	6.937	61.938	29.742	164.199			
5200	6.955	62.073	30.363	164.894			
5300	6.973	62.206	30.963	165.590			
5400	6.992	62.336	31.542	166.288			
5500	7.011	62.465	32.104	166.988			
5600	7.030	62.591	32.646	167.691			
5700	7.051	62.716	33.173	168.395			
5800	7.072	62.838	33.683	169.101			
5900	7.093	62.960	34.179	169.809			
6000	7.115	63.079	34.659	170.519			

RHODIUM REFERENCE STATE

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± .070	± .050	± .050	± .000			
1000	± .100	± .110	± .070	± .040			
2000	± .200	± .220	± .120	± .190			
2239	± .200	± .240	± .140	± .230			
2239	± .500	± .600	± .140	± 1.030			
3000	± 2.000	± .960	± .300	± 1.980			
3995.89	± 4.000	± 1.820	± .580	± 4.970			
3995.89	± .001	± .003	± .003	± .002			
5000	± .001	± .003	± .003	± .002			
6000	± .001	± .003	± .003	± .003			

Summary of Basic Data

Solid has face-centered cubic (A1 type) of structure.

m.p. = 2239° ± 3°K
ΔH_m = 5150 ± 800 cal/gfw
ΔS_m = 2.300 ± .360 e.u./gfw

b.p. = 3996° ± 130°K
ΔH_v = 118.145 ± 6.570 Kcal/gfw
ΔS_v = 29.563 ± 2.693 e.u./gfw

S_{298}° = 7.530 ± .050 e.u./gfw $H_{298}^\circ - H_0^\circ$ = 1174 cal/gfw   gfw = 102.91

$C_{p(\text{solid})}^\circ = 5.600 + 2.020 \times 10^{-3}T - 0.2334 \times 10^{5}T^{-2}$ (cal/°K gfw)

$C_{p(\text{liquid})}^\circ$ = 10.000 cal/°K gfw

TABLE VI - 23

RHODIUM — IDEAL MONATOMIC GAS — Rh

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid from 0° to 2239°K,
Liquid from 2239° to 3996°K, Gas from 3996° to 6000°K.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-1.483	132.461	132.461	Infinite
298.15	5.023	44.388	44.388	0.000	132.770	121.781	-89.264
300	5.025	44.419	44.388	0.009	132.768	121.713	-88.664
400	5.174	45.883	44.587	0.518	132.666	118.042	-64.492
500	5.386	47.060	44.967	1.046	132.554	114.398	-50.001
600	5.618	48.062	45.402	1.596	132.441	110.778	-40.349
700	5.839	48.945	45.846	2.169	132.328	107.177	-33.461
800	6.034	49.738	46.284	2.763	132.215	103.591	-28.298
900	6.198	50.458	46.708	3.375	132.099	100.021	-24.287
1000	6.329	51.118	47.117	4.002	131.977	96.463	-21.081
1100	6.430	51.727	47.508	4.640	131.844	92.918	-18.460
1200	6.505	52.290	47.884	5.287	131.701	89.384	-16.278
1300	6.558	52.812	48.243	5.940	131.543	85.865	-14.435
1400	6.594	53.300	48.587	6.598	131.369	82.359	-12.856
1500	6.617	53.756	48.917	7.259	131.179	78.863	-11.490
1600	6.629	54.183	49.232	7.921	130.968	75.383	-10.296
1700	6.635	54.585	49.536	8.584	130.739	71.913	-9.245
1800	6.636	54.965	49.827	9.248	130.490	68.461	-8.312
1900	6.634	55.323	50.107	9.911	130.220	65.024	-7.479
2000	6.631	55.663	50.376	10.575	129.931	61.600	-6.731
2100	6.626	55.987	50.636	11.237	129.619	58.191	-6.056
2200	6.623	56.295	50.886	11.900	129.289	54.798	-5.443
2239	6.622	56.410	50.980	12.158	129.154	53.480	-5.220
2239	6.622	56.410	50.980	12.158	124.004	53.480	-5.220
2300	6.620	56.589	51.128	12.562	123.798	51.557	-4.899
2400	6.618	56.871	51.361	13.224	123.460	48.424	-4.409
2500	6.618	57.141	51.587	13.886	123.122	45.305	-3.960
2600	6.620	57.401	51.806	14.548	122.784	42.199	-3.547
2700	6.623	57.651	52.017	15.210	122.446	39.107	-3.165
2800	6.627	57.892	52.223	15.872	122.108	36.027	-2.812
2900	6.634	58.124	52.422	16.535	121.771	32.961	-2.484
3000	6.641	58.349	52.616	17.199	121.435	29.903	-2.178
3100	6.650	58.567	52.805	17.864	121.100	26.855	-1.893
3200	6.660	58.779	52.988	18.529	120.765	23.820	-1.627
3300	6.671	58.984	53.167	19.196	120.432	20.794	-1.377
3400	6.683	59.183	53.341	19.863	120.099	17.782	-1.143
3500	6.695	59.377	53.511	20.532	119.768	14.774	-0.922
3600	6.708	59.566	53.676	21.202	119.438	11.781	-0.715
3700	6.721	59.750	53.838	21.874	119.110	8.794	-0.519
3800	6.735	59.929	53.996	22.547	118.783	5.820	-0.335
3900	6.749	60.104	54.150	23.221	118.457	2.849	-0.160
3995.89	6.763	60.269	54.295	23.872	118.145	0.000	0.000
3995.89	6.763	60.269	54.295	23.872			
4000	6.764	60.275	54.301	23.897			
4100	6.778	60.442	54.449	24.574			
4200	6.793	60.606	54.594	25.252			
4300	6.808	60.766	54.735	25.932			
4400	6.823	60.923	54.874	26.614			
4500	6.839	61.076	55.010	27.297			
4600	6.854	61.227	55.144	27.982			
4700	6.870	61.374	55.275	28.668			
4800	6.887	61.519	55.403	29.356			
4900	6.903	61.661	55.530	30.045			
5000	6.920	61.801	55.654	30.736			
5100	6.937	61.938	55.775	31.429			
5200	6.955	62.073	55.895	32.124			
5300	6.973	62.206	56.013	32.820			
5400	6.992	62.336	56.129	33.518			
5500	7.011	62.465	56.243	34.218			
5600	7.030	62.591	56.355	34.921			
5700	7.051	62.716	56.466	35.625			
5800	7.072	62.838	56.575	36.331			
5900	7.093	62.960	56.682	37.039			
6000	7.115	63.079	56.787	37.749			

RHODIUM IDEAL MONATOMIC GAS

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± .000	± .002	± .002	± .000	± 1.600	± 1.620	± 1.190
1000	± .001	± .002	± .003	± .000	± 1.640	± 1.670	± .360
2000	± .001	± .003	± .003	± .001	± 1.790	± 1.850	± .200
2239	± .001	± .003	± .003	± .001	± 1.830	± 1.920	± .190
2239	± .001	± .003	± .003	± .001	± 2.630	± 1.920	± .190
3000	± .001	± .003	± .003	± .001	± 3.580	± 2.520	± .180
3995.89	± .001	± .003	± .003	± .001	± 6.570	± 3.930	± .210
3995.89	± .001	± .003	± .003	± .002			
4000	± .001	± .003	± .003	± .002			
5000	± .001	± .003	± .003	± .002			
6000	± .001	± .003	± .003	± .003			

Summary of Basic Data

S_{298}° = 44.388 e.u./gfw

$H_{298}^\circ - H_0^\circ$ = 1483 cal/gfw

ΔH_{f298}° = 132.770 ± 1.600 Kcal/gfw

gfw = 102.91

Spectroscopic energy levels from Moore, C., Nat. Bur. Stds. Circular 467, Vol. 3 (1 May 1958).

TABLE VI - 24

TECHNETIUM REFERENCE STATE Tc

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid from 0° to 2473°K, Liquid from 2473° to 4840°K, Gas from 4840° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
0	0.000	0.000	Infinite	-1.230			
298.15	5.800	8.000	8.000	0.000			
300	5.804	8.036	8.000	0.011			
400	6.004	9.733	8.230	0.601			
500	6.204	11.094	8.671	1.212			
600	6.404	12.243	9.173	1.842			
700	6.604	13.245	9.685	2.492			
800	6.804	14.140	10.187	3.163			
900	7.004	14.953	10.672	3.853			
1000	7.204	15.701	11.138	4.564			
1100	7.404	16.397	11.585	5.294			
1200	7.604	17.050	12.013	6.044			
1300	7.804	17.667	12.425	6.815			
1400	8.004	18.252	12.820	7.605			
1500	8.204	18.811	13.201	8.416			
1600	8.404	19.347	13.569	9.246			
1700	8.604	19.863	13.924	10.096			
1800	8.804	20.360	14.268	10.967			
1900	9.004	20.842	14.601	11.857			
2000	9.204	21.309	14.925	12.768			
2100	9.404	21.762	15.240	13.698			
2200	9.604	22.204	15.546	14.648			
2300	9.804	22.636	15.845	15.619			
2400	10.004	23.057	16.137	16.609			
2473	10.150	23.359	16.346	17.345			
2473	10.000	25.659	16.346	23.033			
2500	10.000	25.768	16.447	23.303			
2600	10.000	26.160	16.813	24.303			
2700	10.000	26.538	17.166	25.303			
2800	10.000	26.901	17.507	26.303			
2900	10.000	27.252	17.837	27.303			
3000	10.000	27.591	18.157	28.303			
3100	10.000	27.919	18.466	29.303			
3200	10.000	28.236	18.767	30.303			
3300	10.000	28.544	19.058	31.303			
3400	10.000	28.843	19.342	32.303			
3500	10.000	29.133	19.618	33.303			
3600	10.000	29.414	19.886	34.303			
3700	10.000	29.688	20.147	35.303			
3800	10.000	29.955	20.402	36.303			
3900	10.000	30.215	20.650	37.303			
4000	10.000	30.468	20.892	38.303			
4100	10.000	30.715	21.129	39.303			
4200	10.000	30.956	21.360	40.303			
4300	10.000	31.191	21.586	41.303			
4400	10.000	31.421	21.807	42.303			
4500	10.000	31.646	22.023	43.303			
4600	10.000	31.866	22.234	44.303			
4700	10.000	32.081	22.442	45.303			
4800	10.000	32.291	22.645	46.303			
4840.07	10.000	32.374	22.724	46.704			
4840.07	7.499	61.273	22.724	186.575			
4900	7.522	61.366	23.198	187.024			
5000	7.559	61.518	23.962	187.778			
5100	7.594	61.668	24.700	188.536			
5200	7.628	61.816	25.413	189.297			
5300	7.660	61.961	26.100	190.061			
5400	7.691	62.105	26.766	190.829			
5500	7.720	62.246	27.410	191.600			
5600	7.748	62.386	28.034	192.373			
5700	7.774	62.523	28.637	193.149			
5800	7.798	62.658	29.222	193.928			
5900	7.821	62.792	29.790	194.709			
6000	7.842	62.923	30.341	195.492			

TECHNETIUM REFERENCE STATE

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± .100	± .500	± .500	± .000			
1000	± .500	± .740	± .600	± .140			
2000	± 1.000	± 1.260	± .600	± .890			
2473	± 1.250	± 1.500	± .810	± 1.420			
2473	± .500	± 1.900	± .920	± 2.420			
3000	± 1.550	± 2.100	± .920	± 2.960			
4000	± 3.550	± 2.830	± 1.110	± 4.510			
4840.07	± 5.230	± 3.670	± 1.700	± 8.200			
4840.07	± .001	± .003	± .003	± 002			
5000	± .001	± .003	± 003	± .002			
6000	± .001	± .003	± .003	± .003			

Summary of Basic Data

Solid has hexagonal close packed (A3 type) structure.

m.p. = $2473^\circ \pm 50^\circ$K

b.p. = $4840^\circ \pm 500^\circ$K

ΔH_m = 5688 ± 1000 cal/gfw

ΔH_v = 139.871 ± 13.200 Kcal/gfw

ΔS_m = 2.300 ± .400 e.u./gfw

ΔS_v = 28.899 ± 6.371 e.u./gfw

S_{298}° = 8.000 ± .500 e.u./gfw

$H_{298}^\circ - H_0^\circ$ = 1230 cal/gfw

gfw = 99*

$C_{p(\text{solid})}^\circ = 5.200 + 2.000 \times 10^{-3}T$ (cal/°K gfw)

$C_{p(\text{liquid})}^\circ$ = 10.000 cal/°K gfw

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* Isotope of longest known half-life

TABLE VI - 25

TECHNETIUM IDEAL MONATOMIC GAS Tc

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid from 0° to 2473°K,
Liquid from 2473° to 4840°K, Gas from 4840° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	Infinite	-1.481	154.749	154.749	Infinite
298.15	4.970	43.250	43.250	0.000	155.000	144.490	-105.904
300	4.970	43.280	43.250	0.009	154.998	144.425	-105.208
400	4.999	44.713	43.445	0.507	154.906	140.914	-76.988
500	5.106	45.838	43.815	1.012	154.800	137.428	-60.067
600	5.328	46.787	44.233	1.532	154.690	133.964	-48.794
700	5.660	47.632	44.659	2.081	154.589	130.518	-40.748
800	6.060	48.413	45.080	2.667	154.504	127.086	-34.717
900	6.477	49.151	45.492	3.294	154.441	123.662	-30.028
1000	6.863	49.854	45.893	3.961	154.397	120.245	-26.278
1100	7.184	50.524	46.284	4.664	154.370	116.831	-23.211
1200	7.424	51.160	46.664	5.395	154.351	113.419	-20.655
1300	7.581	51.761	47.033	6.146	154.331	110.010	-18.493
1400	7.663	52.326	47.391	6.909	154.304	106.601	-16.640
1500	7.683	52.856	47.738	7.677	154.261	103.194	-15.035
1600	7.657	53.351	48.074	8.444	154.198	99.792	-13.630
1700	7.597	53.814	48.398	9.207	154.111	96.394	-12.392
1800	7.517	54.246	48.711	9.963	153.996	93.003	-11.292
1900	7.426	54.650	49.013	10.710	153.853	89.617	-10.308
2000	7.332	55.028	49.304	11.448	153.680	86.242	-9.424
2100	7.241	55.384	49.585	12.176	153.478	82.876	-8.625
2200	7.156	55.718	49.857	12.896	153.248	79.516	-7.899
2300	7.080	56.035	50.118	13.608	152.989	76.172	-7.238
2400	7.015	56.335	50.371	14.313	152.704	72.838	-6.632
2473	6.974	56.543	50.549	14.823	152.478	70.416	-6.223
2473	6.974	56.543	50.549	14.823	146.790	70.416	-6.223
2500	6.961	56.620	50.615	15.011	146.708	69.580	-6.082
2600	6.918	56.892	50.852	15.705	146.402	66.499	-5.590
2700	6.887	57.153	51.080	16.395	146.092	63.432	-5,134
2800	6.866	57.403	51.302	17.083	145.780	60.374	-4.712
2900	6.856	57.643	51.516	17.769	145.466	57.331	-4.320
3000	6.854	57.876	51.724	18.454	145.151	54.299	-3.955
3100	6.860	58.101	51.926	19.140	144.837	51.274	-3.615
3200	6.874	58.319	52.123	19.827	144.524	48.261	-3.296
3300	6.894	58.530	52.314	20.515	144.212	45.255	-2.997
3400	6.920	58.737	52.500	21.206	143.903	42.263	-2.717
3500	6.950	58.938	52.681	21.899	143.596	39.280	-2.453
3600	6.984	59.134	52.857	22.596	143.293	36.304	-2.204
3700	7.021	59.326	53.030	23.296	142.993	33.333	-1.969
3800	7.061	59.513	53.198	24.000	142.697	30.375	-1.747
3900	7.102	59.697	53.362	24.708	142.405	27.423	-1.537
4000	7.144	59.878	53.523	25.420	142.117	24.476	-1.337
4100	7.188	60.055	53.680	26.137	141.834	21.541	-1.148
4200	7.231	60.228	53.834	26.858	141.555	18.609	-0.968
4300	7.275	60.399	53.984	27.583	141.280	15.689	-0.797
4400	7.318	60.567	54.132	28.313	141.010	12.770	-0.634
4500	7.361	60.732	54.277	29.047	140.744	9.857	-0.479
4600	7.403	60.894	54.419	29.785	140.482	6.949	-0.330
4700	7.444	61.054	54.558	30.528	140.225	4.055	-0.189
4800	7.484	61.211	54.695	31.274	139.971	1.160	-0.053
4840.07	7.499	61.273	54.749	31.575	139.871	0.000	0.000
4840.07	7.499	61.273	54.749	31.575			
4900	7.522	61.366	54.830	32.024			
5000	7.559	61.518	54.962	32.778			
5100	7.594	61.668	55.092	33.536			
5200	7.628	61.816	55.220	34.297			
5300	7.660	61.961	55.346	35.061			
5400	7.691	62.105	55.470	35.829			
5500	7.720	62.246	55.592	36.600			
5600	7.748	62.386	55.712	37.373			
5700	7.774	62.523	55.830	38.149			
5800	7.798	62.658	55.947	38.928			
5900	7.821	62.792	56.062	39.709			
6000	7.842	62.923	56.175	40.492			

TECHNETIUM IDEAL MONATOMIC GAS

Summary of Uncertainty Estimates

T, °K	cal/°K gfw			Kcal/gfw			
	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
298.15	± .000	± .002	± .002	± .000	± 5.000	± 5.150	± 3.770
1000	± .001	± .002	± .002	± .000	± 5.140	± 5.600	± 1.220
2000	± .001	± .003	± .003	± .001	± 5.890	± 6.630	± .720
2473	± .001	± .003	± .003	± .001	± 6.420	± 7.280	± .640
2473	± .001	± .003	± .003	± .001	± 7.420	± 7.280	± .640
3000	± .001	± .003	± .003	± .001	± 7.960	± 8.340	± .610
4000	± .001	± .003	± .003	± 002	± 9.510	± 11.810	± .650
4840.07	± .001	± .003	± .003	± .002	± 13.200	± 14.600	± .660
4840.07	± .001	± .003	± .003	± .002			
5000	± .001	± .003	± .003	± .002			
6000	± .001	± .003	± .003	± .003			

Summary of Basic Data

S^o_{298} = 43.250 e.u./gfw

$H^o_{298}-H^o_0$ = 1481 cal/gfw

ΔH^o_{f298} = 155.000 ± 5.000 Kcal/gfw

gfw = 99[*]

Spectroscopic energy levels from Moore, C., Nat. Bur. Stds. Circular 467, Vol. 3 (1 May 1958).

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[*] Isotope of longest known half-life.

TABLE VI - 26

THORIUM REFERENCE STATE Th

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid from 0° to 2028°K, Liquid from 2028° to 5060°K, Gas from 5060° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
0	0.000	0.000	Infinite	-1.556			
298.15	6.532	12.760	12.760	0.000			
300	6.537	12.800	12.760	0.012			
400	6.792	14.716	13.020	0.679			
500	7.047	16.259	13.518	1.370			
600	7.302	17.566	14.086	2.088			
700	7.557	18.711	14.667	2.831			
800	7.812	19.737	15.238	3.599			
900	8.067	20.671	15.790	4.393			
1000	8.368	21.536	16.322	5.214			
1100	8.730	22.350	16.833	6.068			
1200	9.170	23.128	17.325	6.963			
1300	9.702	23.882	17.801	7.906			
1400	10.341	24.624	18.262	8.907			
1500	11.104	25.362	18.710	9.978			
1600	12.001	26.107	19.150	11.132			
1633	12.338	26.356	19.293	11.533			
1633	11.000	26.756	19.293	12.186			
1700	11.000	27.198	19.596	12.923			
1800	11.000	27.827	20.036	14.023			
1900	11.000	28.422	20.462	15.123			
2000	11.000	28.986	20.874	16.223			
2028	11.000	29.139	20.987	16.531			
2028	11.000	31.039	20.987	20.384			
2100	11.000	31.422	21.339	21.176			
2200	11.000	31.934	21.809	22.276			
2300	11.000	32.423	22.260	23.376			
2400	11.000	32.891	22.693	24.476			
2500	11.000	33.340	23.110	25.576			
2600	11.000	33.772	23.512	26.676			
2700	11.000	34.187	23.899	27.776			
2800	11.000	34.587	24.274	28.876			
2900	11.000	34.973	24.636	29.976			
3000	11.000	35.346	24.987	31.076			
3100	11.000	35.707	25.327	32.176			
3200	11.000	36.056	25.657	33.276			
3300	11.000	36.394	25.977	34.376			
3400	11.000	36.723	26.289	35.476			
3500	11.000	37.042	26.591	36.576			
3600	11.000	37.351	26.886	37.676			
3700	11.000	37.653	27.173	38.776			
3800	11.000	37.946	27.452	39.876			
3900	11.000	38.232	27.725	40.976			
4000	11.000	38.510	27.991	42.076			
4100	11.000	38.782	28.251	43.176			
4200	11.000	39.047	28.505	44.276			
4300	11.000	39.306	28.753	45.376			
4400	11.000	39.559	28.996	46.476			
4500	11.000	39.806	29.234	47.576			
4600	11.000	40.048	29.466	48.676			
4700	11.000	40.284	29.693	49.776			
4800	11.000	40.516	29.917	50.876			
4900	11.000	40.743	30.136	51.976			
5000	11.000	40.965	30.350	53.076			
5060.26	11.000	41.097	30.477	53.739			
5060.26	9.340	65.357	30.477	176.504			
5100	9.356	65.430	30.749	176.875			
5200	9.394	65.612	31.417	177.812			
5300	9.430	65.792	32.065	178.753			
5400	9.464	65.968	32.691	179.698			
5500	9.496	66.142	33.297	180.646			
5600	9.525	66.314	33.886	181.597			
5700	9.552	66.482	34.456	182.551			
5800	9.575	66.649	35.010	183.507			
5900	9.596	66.813	35.548	184.466			
6000	9.613	66.974	36.070	185.426			

THORIUM REFERENCE STATE

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± .050	± .200	± .200	± .000			
1000	± .150	± .260	± .220	± .040			
1633	± .250	± .360	± .260	± .160			
1633	± 1.000	± .480	± .260	± .360			
2028	± 1.000	± .700	± .320	± .760			
2028	± .600	± 1.190	± .320	± 1.760			
3000	± 2.800	± 1.860	± .720	± 3.410			
4000	± 5.000	± 2.980	± 1.150	± 7.310			
5060.26	± 7.300	± 4.420	± 1.690	± 13.830			
5060.26	± .500	± .465	± .220	± 1.230			
6000	± .600	± .575	± .280	± 1.780			

Summary of Basic Data

Solid has two modifications:

$$\alpha \overset{I}{\rightleftharpoons} \beta$$

has face-centered cubic (A1 type) structure.
has body-centered cubic (A2 type) structure.

Transition	I	m.p.	b.p.
Temperature °K	1633	2028	5060° ± 440°K
ΔH (Kcal/gfw)	0.653 ± .200	3.853 ± 1.000	122.765 ± 15.060
ΔS (e.u./gfw)	0.400 ± .120	1.900 ± .490	24.260 ± 5.570

$S_{298}^\circ = 12.760 \pm .200$ e.u./gfw $H_{298}^\circ - H_0^\circ = 1556$ cal/gfw gfw = 232.05

$C_p^\circ(\alpha, 298^\circ \text{ to } 800^\circ K) = 5.773 + 2.548 \times 10^{-3}T$ (cal/°K gfw)

$C_p^\circ(\alpha, 800^\circ \text{ to } 1633^\circ K) = 5.553 + 4.928 \times 10^{-3}T - 4.703 \times 10^{-6}T^2$

$C_p^\circ(\beta, 1633^\circ K \text{ to m.p.}) = 11.000$ cal/°K gfw

C_p°(liquid) = 11.000 cal/°K gfw

TABLE VI - 27

THORIUM IDEAL MONATOMIC GAS Th

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid from 0° to 2028°K, Liquid from 2028° to 5060°K, Gas from 5060° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
0	0.000	0.000	Infinite	-1.481	137.775	137.775	Infinite
298.15	4.969	45.426	45.426	0.000	137.700	127.961	-93.793
300	4.969	45.457	45.426	0.009	137.697	127.900	-93.171
400	4.982	46.888	45.621	0.506	137.527	124.660	-68.108
500	5.039	48.004	45.990	1.007	137.337	121.464	-53.089
600	5.171	48.934	46.405	1.517	137.129	118.309	-43.092
700	5.388	49.746	46.826	2.044	136.913	115.189	-35.962
800	5.679	50.484	47.237	2.597	136.698	112.101	-30.623
900	6.022	51.172	47.637	3.182	136.489	109.038	-26.477
1000	6.390	51.825	48.023	3.802	136.288	105.999	-23.165
1100	6.761	52.452	48.398	4.460	136.092	102.978	-20.459
1200	7.116	53.056	48.761	5.154	135.891	99.977	-18.207
1300	7.441	53.638	49.114	5.882	135.676	96.993	-16.305
1400	7.729	54.201	49.457	6.641	135.434	94.027	-14.678
1500	7.975	54.742	49.791	7.426	135.148	91.078	-13.269
1600	8.180	55.264	50.117	8.235	134.803	88.153	-12.041
1633	8.240	55.432	50.222	8.508	134.675	87.193	-11.669
1633	8.240	55.432	50.222	8.508	134.022	87.193	-11.669
1700	8.346	55.765	50.435	9.061	133.838	85.274	-10.962
1800	8.476	56.246	50.744	9.903	133.580	82.426	-10.007
1900	8.574	56.707	51.046	10.755	133.332	79.590	-9.155
2000	8.646	57.149	51.340	11.616	133.093	76.768	-8.388
2028	8.661	57.268	51.420	11.859	133.028	75.982	-8.188
2028	8.661	57.268	51.420	11.859	129.175	75.982	-8.188
2100	8.695	57.572	51.627	12.484	129.008	74.095	-7.711
2200	8.727	57.977	51.907	13.355	128.779	71.484	-7.101
2300	8.745	58.365	52.179	14.229	128.553	68.886	-6.545
2400	8.754	58.738	52.445	15.104	128.328	66.295	-6.037
2500	8.755	59.095	52.703	15.979	128.103	63.718	-5.570
2600	8.751	59.438	52.956	16.854	127.878	61.146	-5.140
2700	8.746	59.769	53.202	17.729	127.653	58.582	-4.742
2800	8.740	60.087	53.442	18.604	127.428	56.030	-4.373
2900	8.735	60.393	53.677	19.477	127.201	53.481	-4.030
3000	8.732	60.687	53.906	20.351	126.975	50.943	-3.711
3100	8.732	60.976	54.129	21.224	126.748	48.414	-3.413
3200	8.735	61.253	54.347	22.097	126.521	45.892	-3.134
3300	8.742	61.522	54.561	22.971	126.295	43.373	-2.872
3400	8.754	61.783	54.769	23.846	126.070	40.868	-2.627
3500	8.769	62.037	54.973	24.722	125.846	38.363	-2.395
3600	8.789	62.284	55.173	25.600	125.624	35.867	-2.177
3700	8.812	62.525	55.369	26.480	125.404	33.375	-1.971
3800	8.839	62.761	55.560	27.362	125.186	30.890	-1.776
3900	8.870	62.991	55.748	28.247	124.971	28.410	-1.592
4000	8.903	63.216	55.931	29.136	124.760	25.940	-1.417
4100	8.940	63.436	56.112	30.028	124.552	23.470	-1.251
4200	8.978	63.652	56.289	30.924	124.348	21.007	-1.093
4300	9.018	63.863	56.462	31.824	124.148	18.551	-0.943
4400	9.060	64.071	56.633	32.728	123.952	16.097	-0.799
4500	9.103	64.275	56.801	33.636	123.760	13.648	-0.663
4600	9.146	64.476	56.965	34.548	123.572	11.205	-0.532
4700	9.189	64.673	57.127	35.465	123.389	8.760	-0.407
4800	9.232	64.867	57.286	36.386	123.210	6.329	-0.288
4900	9.275	65.058	57.443	37.312	123.036	3.896	-0.174
5000	9.316	65.245	57.597	38.241	122.865	1.465	-0.064
5060.26	9.340	65.357	57.689	38.804	122.765	0.000	0.000
5060.26	9.340	65.357	57.689	38.804			
5100	9.356	65.430	57.749	39.175			
5200	9.394	65.612	57.899	40.112			
5300	9.430	65.792	58.046	41.053			
5400	9.464	65.968	58.191	41.998			
5500	9.496	66.142	58.334	42.946			
5600	9.525	66.314	58.475	43.897			
5700	9.552	66.482	58.614	44.851			
5800	9.575	66.649	58.751	45.807			
5900	9.596	66.813	58.886	46.766			
6000	9.613	66.974	59.020	47.726			

THORIUM IDEAL MONATOMIC GAS

Summary of Uncertainty Estimates

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
298.15	± .010	± .005	± .005	± .000	± 1.000	± 1.060	± .780
1000	± .100	± .059	± .027	± .032	± 1.070	± 1.250	± .270
1633	± .160	± .120	± .050	± .120	± .280	± 1.510	± .200
1633	± .160	± .120	± .050	± .120	± .480	± 1.510	± .200
2028	± .200	± .160	± .070	± .180	± .940	± 1.790	± .190
2028	± .200	± .160	± .070	± .180	± 1.940	± 1.790	± .190
3000	± .300	± .260	± .120	± .430	± 3.840	± 3.520	± .260
4000	± .400	± .365	± .170	± .780	± 8.090	± 6.280	± .340
5060.26	± .500	± .465	± .220	± 1.230	± 15.060	± 10.660	± .460
5060.26	± .500	± .465	± .220	± 1.230			
6000	± .600	± .575	± .280	± 1.780			

Summary of Basic Data

S_{298}° = 45.426 ± .005 3.u. /gfw

$H_{298}^\circ - H_0^\circ$ = 1481 cal/gfw

ΔH_{f298}° = 137.700 ± 1.000 Kcal/gfw

gfw = 232.05

Spectroscopic energy levels from Zalubas, R., J. Res. Natl. Bur. Stds. 63A, 275 (1959).

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