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NATIONAL BUREAU OF STANDARDS REPORT

8628

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

(Supplement to NBS Reports 6297, 6484, 6645, 6928, 7093, 7192, 7437, 7587, 7796, 8033, 8166, and 8504)

1 January 1965

NBS

U.S. DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

THE NATIONAL BUREAU OF STANDARDS

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NBS REPORT

8628

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

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Thirteenth Technical Summary Report
on the Thermodynamic Properties
of Light-Element Compounds

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ABSTRACT

This is the thirteenth semiannual report on the current experimental, theoretical, and evaluative program, at the National Bureau of Standards, on the thermodynamic properties of selected light-element and some related compounds of primary interest in high-temperature research. Included are new experimental results in several areas; and a number of tables of thermodynamic functions, heats of formation, ionization potentials, and electron affinities resulting from literature surveys and critical data evaluations.

New experimental work on the borohydrides of aluminum and beryllium is reported. The mean value found for the standard heat of formation of $A\ell(BH_4)_3$ (298°K) is +2 kcal/mole for the gas and -5 kcal/mole for the liquid, with an estimated possible error as great as 17 kcal/mole. The infrared spectra of MgF_2 (in a krypton matrix), $A\ell(BH_4)_3$, and $Be(BH_4)_2$ were measured, and a new band system was discovered for F_2^+. The bending fundamental of MgF_2 appears to be 242 cm^{-1}, and continuing spectroscopic work is expected to provide additional molecular constants for the other substances. High-temperature mass-spectrometric data on the BeO-$A\ell_2O_3$ system were treated thermodynamically, and lead to heats of atomization for O_2, $A\ell_2O$, and the new molecule $A\ell OBe$ (as well as the heat of vaporization of liquid $BeO \cdot A\ell_2O_3$). The values for O_2 and $A\ell_2O$ agree well with previously available values. Recent precise measurements of the relative enthalpy of graphite over the range 1200-2600°K are summarized. Liquid $A\ell_2O_3$ was vaporized in vacuum and the condensates subjected to varying programs of annealing. The progress from amorphous to the stable alpha crystalline form was followed in detail by X-ray and electron diffraction.

The report includes four appendices. The first is a formula-property index of the twelve preceding semiannual reports. The second comprises new tables of the standard thermodynamic properties of condensed phases of 17 substances, including 13 "mixed" oxides. The third appendix gives thermochemical values for additional compounds of several elements which have resulted from a current revision of NBS Circular 500 (Series I). The fourth appendix includes the table of ionization potentials and electron affinities of light-element atoms and molecules presented in the last report but now considerably revised and augmented by recent information.

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Project Leader

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B-119	CaC_2	Solid(α,β)	0-1500	54
B-120	$3CaO \cdot A\ell_2O_3$	Solid	0-1800	56
B-121	$12CaO \cdot 7A\ell_2O_3$	Solid(α,β)	0-1800	58
B-122	$CaO \cdot A\ell_2O_3$	Solid	0-1800	60
B-123	$CaO \cdot 2A\ell_2O_3$	Solid	0-1800	62
B-124	$3CaO \cdot 2SiO_2$	Solid	0-300	64
B-125	$2CaO \cdot SiO_2$	Solid(γ)	0-1120	65
B-126	$2CaO \cdot SiO_2$	Solid(β,α',α)	0-2000	67
B-127	$CaO \cdot Fe_2O_3$	Solid and Liquid	0-2000	69
B-128	$2CaO \cdot Fe_2O_3$	Solid and Liquid	0-2000	71
B-129	$CoO \cdot Fe_2O_3$	Solid	0-300	73
B-130	$FeO \cdot Co_2O_3$	Solid	0-300	74
B-131	$NiO \cdot Fe_2O_3$	Solid	0-300	75
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Chapter 1

HEAT OF CHLORINATION OF ALUMINUM BOROHYDRIDE

by A. A. Gilliland and D. D. Wagman

I. Introduction

Aluminum borohydride is a colorless volatile liquid, spontaneously flammable in air, and violently reactive with moisture. It is reported to react with hydrocarbon stopcock lubricants, but is inert with respect to Kel-F grease, although it does apparently dissolve and diffuse slowly through the grease.

Initial attempts to obtain a suitable calorimetric reaction involved bomb reactions with N_2 under pressure, $Cl_2(g)$ and with water vapor. In all cases a mixture of unidentified reaction products were obtained, including strong odors indicating the probable presence of boron hydrides. Attempts to bubble $Al(BH_4)_3$ vapor into dilute hydrochloric acid solutions also failed to produce well-defined products. The reaction that was finally selected was the vapor-phase chlorination using a flow calorimeter designed to maintain a steady flame at the burner tip. The general procedure is similar to that used for the oxygen flame combustion of hydrocarbons [1]. No spark ignition is required as the chlorination reaction proceeds spontaneously.

II. Materials

The sample of $Al(BH_4)_3$ was obtained from the Union Carbide and Carbon Corporation, South Charleston, W. Virginia. It was stored in a steel cylinder at -20°C except during transfer operations. Samples for measurement, approximately 0.4-0.5 g, were transferred by vapor distillation into small glass bulbs and stored in a freezer chest until used.

The only information we have with respect to the purity of the $Al(BH_4)_3$ comes from the analysis of the reaction products as described in the Section on Procedure and shown in Table 2. A small amount of a black solid powder was formed during each calorimetric run and was carried by the gas stream out of the reaction vessel into the collecting line and traps. An analysis of this sample indicated it to contain approximately 15% carbon, and significant amounts of Si, Al, and B. No crystalline structure was detected. Attempts to determine the amount of hydrogen in the sample by evolution as H_2 did not prove satisfactory. Because of the excess of Cl_2 used in the reaction, the amount of HCl formed could not be determined.

Initially the chlorine used was obtained from Matheson Corp. Subsequently a highly purified sample was obtained through the courtesy of Dr. G. Sinke of the Dow Chemical Company, Midland, Michigan. Their analysis indicated a purity of 99.9% for the liquid phase. We were unable to notice any difference resulting from the different chlorine samples.

III. Procedure

The small bulb containing the sample was placed in a special glass vessel containing a glass hammer, flushed with He, and weighed. On shaking, the small bulb was broken and the vessel was placed in the calorimeter gas flow line. The vessel is so constructed that He gas may be allowed to flow through it, carrying the $Al(BH_4)_3$ vapor into the reaction vessel, at the beginning of the reaction period. At the end of the reaction time the He may be diverted around the vessel without removing it from the line.

The reaction vessel consists of a large diameter Pyrex tube 30 mm O.D., through one end of which enter two concentric tubes which form the burner tube. The mixture of borohydride and helium enters through the inner tube; the outer tube carries He gas used to prevent thermal cracking of the borohydride before it reaches the burner tip. A separate inlet tube in the side of the vessel is connected to the Cl_2 supply cylinder.

The exit end of the vessel leads to a glass coil for thermal equilibration of the product gases with the calorimeter water. The gases then pass through two large traps cooled with liquid N_2 to condense the BCl_3 and HCl produced in the reaction as well as the excess Cl_2. A small amount of $AlCl_3$ is occasionally found in the second trap (possibly carried over by the solid residue previously mentioned); some BCl_3 is also retained on the $AlCl_3$ in the reaction vessel.

When the calorimetric measurement is completed, the traps are connected to two bubblers in series, each containing about 300 ml of H_2O. Upon removal of the liquid N_2, the condensed HCl, Cl_2 and BCl_3 volatilize and bubble through the water, the excess Cl_2 being vented to the outdoors.

After the traps are emptied, the bubblers are titrated for H_3BO_3 produced by the hydrolysis of the BCl_3. The calorimeter vessel, exit tubes and the N_2-traps are washed with water. The washings are combined and four aliquots taken. In two, $Al(OH)_3$ is precipitated by adjusting to pH = 7, filtered, and the H_3BO_3 remaining in the filtrate determined by titration using Mannitol. The total amount of BCl_3 produced is obtained by combining the amount determined here with that found in the bubblers.

In the remaining aliquots, the Al is determined by precipitation as the 8-hydroxyquinolate.

The weight of $Al(BH_4)_3$ reacted is obtained by weighing the large sample holder before and after the reaction. Because of the tendency of the borohydride vapor to diffuse through the grease, the final weighing usually had to be made rapidly, without waiting for the dissipation of static charge, etc.

IV. Results

Four electrical energy calibration experiments were performed, as indicated in Table 1. Helium gas flowed continually during the measurements, at the same rate as was used during the calorimetric runs.

The results of six calorimetric experiments are given in Tables 2 and 3. The results of several other experiments were discarded because of premature losses of sample, failures in the analytical train, etc. In Table 3, the values of q_{total} have been corrected for the energy supplied by the Cl_2 gas entering the system, the correction amounting to 5-9 joules for the various runs.

The values of ΔHf for $Al(BH_4)_3$ given in Table 3 are based on the following considerations. The weight of borohydride sample is used to calculate the total amount of HCl(g) produced, assuming 12 moles HCl per mole of borohydride. While this stoichiometry is not correct, since a small amount of carbonaceous residue is produced, we assume that metal alkyl impurities are present in the sample and that the heat of chlorination is comparable to that of the $Al(BH_4)_3$. In view of the fact that the solid residue also contained Al and B, the amounts of $AlCl_3$ and BCl_3 formed are computed from the individual analytical results for Al and B respectively, as shown in Table 2. The heats of formation of the HCl, $AlCl_3$(c), and BCl_3 formed are listed in columns 4, 5, and 6 of Table 3, based on the molar values of ΔHf from NBS Circular 500 [2].

On the basis of these assumptions, the value of ΔHf for $Al(BH_4)_3$(g) at 25°C = 8.7±2.8 kj/mole (2·1±0.7 kcal/mole)

It is difficult to assess the validity of the assumptions made for these calculations. However it is possible to make an estimate of their significance. If we were to assume that the sample were of high purity and reacted stoichiometrically, we can obtain from the weights of sample a value of ΔHf° = -14.7±1.6 kcal/mole. On the other hand if we base our measure of the amount of reaction solely on the amount of boron recovered in the analyses, we obtain a value of ΔHf° = +15.9±1.6 kcal.

On the basis of these calculations we believe that the value for ΔHf of $Al(BH_4)_3$(g) is bracketed between the values +16 and -15 kcal/mole but that the most reasonable estimate is about 2 kcal/mole.

The vapor pressure equation of Schlesinger et al. [3] leads to a heat of vaporization of 7.2 kcal/mole at a mean temperature of -10°C. Correcting with an estimated ΔC_p = -15 cal/deg to 25°C yields ΔH_v = 6.7 kcal/mole. This corresponds to a value of ΔHf for $Al(BH_4)_3$(liq) = -5 kcal/mole.

References

1. Prosen, Maron and Rossini, J. Research NBS 42, 269 (1949).

2. NBS Circular 500, Selected Values of Chemical Thermodynamic Properties, Government Printing Office, Washington, D.C. (1952).

3. Schlesinger, Sanderson, and Burg, J. Am. Chem. Soc. 62, 3421 (1940).

Table 1

Results of Electrical Calibration Expts.

Expt. No.	ΔR_c ohms	E J	E_s J/ohm
1	.108695	17,697.06	162,813.9
2	.129058	21,011.14	162,803.8
3	.129036	21,008.07	162,807.8
4	.115310	18,772.90	162,803.7
Mean			162,807.3
Standard deviation of the mean			3.8$_5$

Table 2

Analytical Results on Chlorination Experiments

Expt. No.	Moles $Al(BH_4)_3$ weighed x 10^3	Moles Al found x 10^3	Moles B found as H_3BO_3 x 10^3	% Al	% B
1	5.076	4.944	14.456	97.39	94.94
2	5.955	5.839	17.347	98.06	97.94
3	5.328	5.153	15.394	96.71	96.30
4	6.735	6.520	19.382	96.82	95.93
5	5.594	5.379	16.025	96.16	95.53
6	7.761	7.531	22.213	(97.03)*	95.40

*Based on the average of preceding 5 experiments.

Table 3

Calorimetric Results of Chlorination Experiments

Expt. No.	ΔR_c, Ω	q_{total} kj	q_{HCl} kj	q_{AlCl_3} kj	q_{BCl_3} kj	$-\Delta Hf_{Al(BH_4)_3}$ kj/mole
1	0.092404	15.039	5.624	3.438	5.898	-15.6
2	.109521	17.822	6.597	4.060	7.078	-14.6
3	.096803	15.753	5.903	3.583	6.281	+ 2.6
4	.122494	19.934	7.462	4.534	7.908	- 4.4
5	.101660	16.542	6.197	3.740	6.538	-12.0
6	.141094	22.962	8.599	5.237	9.063	- 8.1

Mean	-8.7 kj (2.1 kcal/mole)
Standard Deviation of mean	2.8 kj (0.7 kcal/mole)

Chapter 2

INFRARED SPECTRUM OF ALUMINUM BOROHYDRIDE AND BERYLLIUM BOROHYDRIDE

By Arthur G. Maki

Introduction

We have measured the infrared spectrum of aluminum borohydride ($Al(BH_4)_3$) and beryllium borohydride ($Be(BH_4)_2$). Ultimately we would hope to be able to improve the assignments for the fundamental vibrational frequencies of the aluminum compound and to make a corresponding set of assignments for the beryllium compound. The present report, however, will be concerned with general observations regarding the spectra which have thus far been obtained. More spectral data will soon be available and at that time more detailed consideration will be given to the assignments.

Aluminum Borohydride

Emery and Taylor[1] have measured the Raman spectrum of $Al(BH_4)_3$ while Price[2] has reported the infrared absorption spectrum. The infrared work of Price was done with a low resolution instrument and it was hoped that higher resolution work would yield information on the band contours. Such information would be very helpful in making assignments.

We have observed the gas phase spectrum of $Al(BH_4)_3$ in the region from 4000 to 325 cm^{-1} with a resolution of about 0.8 cm^{-1}. In addition, the B-H stretching fundamental bands have been observed (from 2400 to 2600 cm^{-1}) on a high resolution instrument capable of resolving two lines 0.08 cm^{-1} apart.

In an ideal situation, a resolution of 0.8 cm^{-1} would be expected to give different band contours for vibrations of different symmetry species. A rough calculation of the geometry of the molecule indicates that parallel bands should have a strong central Q-branch and P- and R-branches separated by about 16 cm^{-1}. Perpendicular bands, however, would be expected to be broad and featureless with a width of about 25 cm^{-1}. Under higher resolution the perpendicular bands would be expected to have a series of lines 0.16 cm^{-1} apart while the P- and R-branches of a parallel band would have a line spacing of 0.30 cm^{-1}.

The observed bands have no resolvable fine structure even under conditions such that lines 0.08 cm^{-1} apart could be easily resolved. This means that the band contours are of no help in making the assignments for $Al(BH_4)_3$. The cause of this difficulty is apparently two-fold. First of all we know that there is at least one low frequency vibration and we can expect several others. As a consequence there will be a fairly large number of molecules in excited vibrational states thus giving rise to so-called hot bands which will overlap the fundamental bands. In addition, the normal isotopic ratio for boron is 18.8% B^{10} and 81.2% B^{11}. Consequently our sample contains 53% $Al(B^{11}H_4)_3$, 37% $AlB^{10}H_4(B^{11}H_4)_2$, 9% $AlB^{11}H_4(B^{10}H_4)_2$, and 1% $Al(B^{10}H_4)_3$. The molecules containing both B^{10} and B^{11} will of course be asymmetric rotors and their vibration-rotation spectrum will be rather complex.

We have also measured the low temperature infrared spectrum of solid $Al(BH_4)_3$. Since the sample was at a temperature near -150°C, the possibility of difference transitions (transitions originating in an excited vibrational state) is eliminated. The fact that the solid and gas phase spectra are very similar indicates that none of the strong absorption bands can be attributed to such difference transitions. The spectrum of solid $Al(BH_4)_3$ has only been obtained from 4000 to 625 cm^{-1}. Future work is planned which will extend the spectrum to longer wavelengths.

Table 1 gives tentative wavenumber measurements for the absorption bands of aluminum borohydride. The Raman measurements of Emery and Taylor are also given.

Beryllium Borohydride

Initial attempts at obtaining the gas phase infrared spectrum have not been successful. The difficulty is caused by the reactivity of this compound. In addition to attacking the usual infrared window materials (NaCl or KBr) we find that it rapidly attacks small amounts of impurities adsorbed on the walls of our absorption cells. At present, however, we feel that these difficulties can be overcome.

In spite of the fact that we were unable to obtain any helpful information from the band contours of the aluminum compound, we have hopes that the gas phase spectrum of the beryllium compound will be of aid in making the vibrational assignments. Since this molecule has fewer atoms and is lighter, it is expected to have fewer low-lying vibrations thus ameliorating the difficulty caused by hot bands. This gain could be off-set, however, if the torsional frequency is lower. The presence of only two boron atoms per molecule also improves the difficulty caused by the mixture of isotopes. Finally, the smaller moment of inertia for the beryllium compound will cause the bands to be more spread out and the band contours should be better defined.

We have obtained the spectrum of solid $Be(BH_4)_2$ at about -150°C. The spectrum of $Be(BH_4)_2$ reported by Price et al[3] seems to be erroneous. Price later reported[2] that $Be(BH_4)_2$ reacts with the window material used in the infrared absorption cells. We have found that diborane is one product of this reaction. The spectrum reported by Price et al is evidently due to diborane and the solid product of the reaction between $Be(BH_4)_2$ and the window material. Since the reaction with the usual window materials is extremely rapid (the reaction goes to completion in times of the order of seconds or less), it is most unlikely that earlier workers could have observed the infrared spectrum of $Be(BH_4)_2$.

The spectrum for solid $Be(BH_4)_2$ is also given in Table 1. As expected there are striking similarities between the spectra of diborane, beryllium borohydride, and aluminum borohydride. As an aid to the assignments, however, we should still like to have the gas phase spectrum of $Be(BH_4)_2$. The band contours of this compound may be of immeasurable help in making the assignments. Work in this direction is continuing. Further work is also planned in order to extend the spectrum of solid $Be(BH_4)_2$ to wavelengths greater than 15 μ.

References

[1] A. R. Emery and R. C. Taylor, Spectrochimica Acta 16, 1455 (1960).

[2] W. C. Price, J. Chem. Phys. 17, 1044 (1949).

[3] W. C. Price, H. C. Longnet-Higgins, B. Rice, and T. F. Young, J. Chem. Phys. 17, 217 (1949).

Table 1

Infrared and Raman Spectra of Aluminum Borohydride and Beryllium Borohydride Given in Wavenumbers (cm^{-1})

$Al(BH_4)_3$			$Be(BH_4)_2$
Raman spectrum of liquid (see Ref. 1)	I.R.-gas	I.R.-solid at -150°C	I.R. absorption of solid at ca. -150°C
	3922 (w)		2515 (m)
	2966 (w)		2455 (m)
	2932 (w)		2340 (s)
	2890 (w)		2110 (s)
	2800 (w)		1998 (w)
2549	2556 (s)	2544 (s)	1553 (s)
	2491 (s)	2474 (s)	1456 (s)
2473 (polarized)			1325 (s)
2226 (w)	2219.6 (w)	2235 (m)	1131 (m)
2069 (polarized)	2070 (w)	2065 (m)	1010 (w)
	2031 (s)	2030 (s)	905 (w)
2010			735 (s)
1925	1930 (w)	1920 (w)	
1884 (w)			
1521 (w)	1523 (broad)	1523 (s)	
1495 (polarized)			
	Overlapped	1455 (s)	
	1420 (broad)	1415 (s)	
1392 (w)			
1149			
1116 (polarized)			
	1112 (s)	1104 (s)	
976	984 (m)	970 (w)	
	764 (w)	774 (m)	
602	607 (s)		
510 (polarized)	-		
318			

w = weak
m = medium
s = strong

CHAPTER 3

TRANSITIONS IN VAPOR-DEPOSITED ALUMINA

by J. J. Diamond and A. L. Dragoo

In the course of vaporization studies in vacuum on a liquid alumina drop at the end of a polycrystalline Al_2O_3 rod, a transparent film developed on the pyrex flask surrounding the sample. When the deposition time exceeded 40 minutes, the film often peeled loose from the surface and tended to curl up evidencing the presence of some strain. The film was subjected to analysis with an x-ray diffractometer and with electron diffraction, neither of which gave any pattern, indicating an "amorphous" film within the limits of detectability.

In addition, petrographic examination showed an isotropic film with a refractive index of 1.614. Its surface area was 0.6 square meters per gram, as determined by N_2 adsorption in B.E.T. equipment. Infrared absorption showed the water band at 2.9μ and several absorption "fringes" because the film was of the same order of thickness as the wave length of the incident radiation. The film was generally transparent from 1 to 8μ; the transmission fell smoothly to 10.5μ and the film was essentially opaque beyond that to 16μ. The material lost about 4% in weight when ignited to 1200°C. The material is thus a slightly hygroscopic, slightly porous, amorphous, essentially unhydrated alumina.

Stumpf et. al. [1] reported that an amorphous phase formed initially upon dehydration of hydrated aluminas, but their material showed a broad band at 4.5Å in contrast to ours which showed none. Amorphous films were reportedly formed on aluminum foils by oxidation in air and in oxygen and by anodization [2,3,4].

The manner of preparing the initial Al_2O_3-form is known to determine the path by which the material transforms to α-Al_2O_3. Since our method of preparing amorphous alumina differed from previous techniques, an investigation was undertaken of the transition of our film to α-Al_2O_3.

Method

To form the film, the end of a polycrystalline Al_2O_3 rod was melted in a vacuum of 1×10^{-6} torr using an A. D. Little arc image furnace, with the arc operated at 150 A. The specimen rod was held near the "cool" end in a spiral of platinum-rhodium wire and supported along the optical axis of the furnace in the middle of a 500-ml. pyrex round-bottomed flask. The specimens used were rods of Morganite alumina, 0.25 and 0.312 inches in diameter. The purity of the material as supplied was determined by emission spectroscopy to be about 99.7-99.9% Al_2O_3, the major impurities being Si, Fe and Ga. The samples were further purified before use to 99.95-99.99% Al_2O_3 by preferential vaporization of the volatile impurities from the molten tip in vacuum.

The flasks were rinsed several times with distilled water and dried in a drying oven at 125°C. Cleaning of the surface with dichromate or nitric acid solutions caused the film to bond too strongly to the flask. Flasks could not be reused after the crop of separated film had been removed because new layers bonded too firmly to the remaining uneven surface.

A sapphire disk, 0.75 inches in diameter, was cleaned in the same manner as the flasks and inserted in a flask during a series of runs to test the effect of the substrate on the formation of the film.

Samples of the film were pulverized in an alumina mortar, examined with x-ray diffractometer for crystallinity and subjected to the following heat treatment:

Sample 1: 700° (16 hours), 800° (16 hours), 900° (16 hours), 1000° (16 hours), 1100° (16-1/2 hours), 1200° (17 hours) and 1300° (6 hours);

Sample 2: 650° (16 hours), 750° (16 hours), 850° (16 hours), 950° (16 hours), 980° (16 hours) and 1200° (24 hours);

Sample 3: at 700° for successive total annealing times of 1/2, 2-1/2, 10-1/2, 16 and 32 hours;

Sample 4: 900° for successive total annealing times of 1/2, 2, 8, 16 and 32 hours;

Sample 5: same as 4 except at 600°C.

The anneals were carried out in an electrically-heated, box-type furnace, and the temperature of the furnace was read from the controller with an uncertainty of ±10°C. X-ray diffraction patterns were obtained after each anneal. As a check on the temperature readings, an additional sample was annealed at 50° intervals beginning at 650° (furnace temperature) for durations of 24 hours, and the temperature was measured with a Pt/Pt-Rh thermocouple. A correction of -30°C was found to be required over the temperature range of 650° to 1050°C. This correction must be applied to the heat treatment temperatures given above.

A thin film was prepared for examination by electron microscopy and diffraction by depositing the film on a section of microscope slide placed inside the flask. Deposition was discontinued once peeling of the film began, and a fragment of the film was mounted in a heating stage of the electron microscope. The film was observed before heating and at 400°, 620°, 630° and 760°. A sample of film obtained from deposition on a sapphire disk was also analyzed without heating the film.

Results

Representative d-spacings and line intensities are illustrated in Fig. 1 for x-ray diffraction analysis. The broad lines have been drawn to correspond with the diffuse peaks of the diffraction pattern. The diffuse lines common at temperatures below 970°C can be ascribed to small crystal size or to crystal imperfection.

A very weak line appeared first at d=1.39Å after anneal of one-half hour at 570°C; lines next appeared at 1.98 and 2.08Å after annealing for a total of 8 hours at 570°C (Fig. 1a). All lines obtained at 570°C were very weak and often nearly indistinguishable from background. The certainty of a line was determined by its presence in more than one pattern.

Sample 3 (annealed at 670°C, corrected) corresponded to Fig. 1a for an annealing time of 2-1/2 hours, except for the absence of the line at 2.08Å. Sample 3 showed a pattern similar to Fig. 1b after 10-1/2 hours at 670° whereas sample 1 showed a less developed stage of this pattern after annealing for 16 hours at 670°. This suggests that the transition to the form of alumina giving the pattern 1b occurs between 660° and 680°C and that sample 3 was above sample 1 in this range of temperature.

The form represented by Fig. 1b was present up to 900° for 16 hours annealing time. Its d-spacings and intensities are compared in Table 1 with those of the delta and theta aluminas reported by Stumpf [5], the delta alumina reported by Rooksby [6] and the results of Jellinek and Fankuchen [7] for alumina gel annealed at 800°C for one hour. Although many of Stumpf's delta and theta lines are absent from our form, his strongest lines are present. However, our transition alumina has a line at 2.39Å which is not present in either the delta or theta forms of Stumpf. The delta form reported by Rooksby shows little correspondence with our form. The d-spacings of Jellinek and Fankuchen correspond with ours for their strongest intensities although their relative intensities differ. Our transition alumina thus approximates most closely a mixture of the delta and theta aluminas reported by Stumpf.

Annealing of the film for 16 hours at 920° or for 32 hours at 870° resulted in the appearance of lines of α-alumina. Disappearance of the transition form was very nearly completed by 1070°. The patterns obtained at 950° and above began to show sharp lines indicating that the grain size was increasing.

Studies of the film were carried out along its edge with the electron microscope where the film was expected to be thinner. Fig. 2a shows the edge of the film (white area) which was deposited on the sapphire disk. Grain sizes in Fig. 2a are estimated to be on the order of 2200Å (28,000 magnification). Heating the film from the glass slide to 630°C produces the appearance of feathering along the edge due to areas of higher transmission having a breadth of ~11000Å (11,000 X).

Table 1

Transition Aluminas

This Expt. 700°, 32 hrs		Stumpf [5] Delta		Stumpf [5] Theta		Rooksby [6]		Jellinek & Fankuchen [7] 800°, 1 hr	
d	I	d	I	d	I	d	I	d	I
						7.97	8		
						6.58	10		
				5.2	3				
		5.02	3			5.07	20		
4.54	2	4.55	3	4.5	6			4.53	8
		4.07	2			4.05	20		
								3.90	4
				3.53	2	3.56	7		
						3.40	10	3.38	4
						3.28	15		
						3.21	10		
						3.03	10		
2.839	4	2.87	4	2.85	8			2.82	8
						2.783	30		
2.732	4	2.73	8	2.72	8	2.737	30		
		2.58	3	2.56	3	2.593	70		
2.444	3	2.43	6	2.43	8	2.457	70		
2.393	2							2.38	24
2.312	2			2.31	6	2.311	40		
2.278	3	2.28	4			2.277	30	2.27	12
				2.24	1				
						2.156	25		
								2.09	4
				2.01	8				
1.974	6	1.99	8			1.989	70	1.98	62
		1.95	3			1.950	65		
		1.91	2	1.91	4				
		1.80	2	1.80	3	1.793	7	1.81	1
				1.73	1	1.701	4	1.70	4
				1.61	2	1.616	10		
						1.602	15	1.60	4
		1.54	4	1.54	6	1.543	10	1.53	12
1.52	1	1.51	3			1.507	20		
		1.49	4	1.49	4				
		1.45	3	1.45	4	1.462	8		
				1.43	1				
		1.40	6	1.40	6	1.407	60	1.40	100
1.394	10	1.39	10	1.39	10	1.392	100		
				1.34	1				
		1.29	2	1.29	3				
		1.26	1	1.26	2	1.250	4		
				1.23	2	1.238	9		
						1.180	4		
				1.14	2	1.134	10		

Heating to a higher temperature caused a fragment of the film to break off and larger crystalline areas to appear.

The film deposited on the glass slide showed no diffraction pattern before heating, faint rings at 620° to 630°C (2c) and sharp rings at 760°C (2d) after the larger crystalline areas had appeared. The film obtained from deposition on the sapphire disk showed one faint ring nearly masked by a diffuse halo (2e). The d-spacings are given in Table 2.

Table 2

Electron Diffraction d-spacings for Al_2O_3 Films

Al_2O_3 on Glass		Al_2O_3 on sapphire
620°-630°C	760°C	no heating
	2.554 α	
	2.379 α	
2.166 α	2.166 α	
1.966 δ or θ	1.966 δ or θ	
	1.374 α	
		1.25 δ or θ
	1.190 α	
1.147 (?) α		

A designation has been placed opposite of each d-spacing to indicate the form of alumina to which it most closely corresponds.

In contrast to the x-ray analysis of the film deposited on glass, the electron diffraction showed a transition of the amorphous film to α-alumina without going through an intermediate form. On the one hand this could arise from different crystallization along the edge as opposed to the bulk of the film. On the other hand, although the film was only exposed to the intense electron beam used for diffraction during short intervals, some beam crystallization may have resulted in the heated film. An effective temperature for the electrons can be estimated to lie between 150° and 400°C, depending on the rate at which the film loses heat to its surroundings. Consequently, the additional heating produced by the beam may have been easily sufficient to cause the transition to α-alumina.

The film which separated from the sapphire disk did not grow epitaxially on the sapphire as evidenced by the small grain size. Although the crystallinity of the substrate appears to have induced some crystallization of the film, the single faint ring of a transition form suggests that the impinging vapor species, primarily Al and O [8], cool too rapidly to form the ordered α-alumina structure and possibly transfer enough energy to the atoms near the surface of the substrate to disrupt them.

The Transition Alumina

Ervin [9] suggested that the strongest line which occurs at 1.39Å in many of the transition aluminas arises because the oxygen atoms are in cubic close-packing and corresponds to the (440) line of the spinel unit cell. He also proposed that the strong line which occurs at 1.985-2.03Å corresponds to the (400) line of the spinel pattern. Our transition alumina had a strong line at 1.974Å, but this may be a combination of the 1.95 and 1.99Å lines of δ-alumina. Ervin explained, on the one hand, the formation of α-alumina directly from the monohydrate, diaspore, on the basis that both contain oxygen atoms in hexagonal close-packing. On the other hand, the monohydrate, boehmite, forms γ-alumina because of a similar cubic close-packing among the oxygen atoms. The aluminum ions are assumed to be randomly distributed among octahedral and tetrahedral interstices in the metastable, transition forms. The transition aluminas result from an increased ordering of the aluminum ions. At a sufficiently high temperature the cubic close-packed oxide lattice shifts to the hexagonal close-packed lattice of corundum.

Plummer [10] carried Ervin's theory a step further in his study of the formation of metastable alumina by rapid cooling of droplets of molten alumina. Rapid quenching of particles of γ- or α-alumina, less than 15μ diameter, melted in an oxy-hydrogen flame, gave almost entirely a mixture of δ- and θ-aluminas. Slow cooling of molten alumina, however, produced α-alumina. A mechanism thus was required which gave the transition alumina in preference to the thermodynamically more stable α-alumina. He suggested that tetrahedral (T) and octahedral (O) groups of oxygen atoms tend to exist longer in the liquid due to their symmetry and mass and are held together by the more mobile aluminum atoms. At high temperatures, the T-groups are in the majority. If the melt cools rapidly, the aluminum atoms in T-holes will direct new aluminum atoms to positions above O-holes. These in turn will cause the next group of oxygen atoms to take the O-sites creating a spinel structure. If cooling proceeds slowly, the aluminum atoms have time to rearrange and oxygen groups are directed to sites above T-holes resulting in hexagonal close-packing.

The formation of the transition aluminas, which are metastable with respect to α-alumina, from the amorphous film possibly follows a mechanism similar to that outlined by Plummer. The oxygen atoms first group into T-groups with most of the aluminum ions in T-holes. These groups of oxygen are bound together by aluminum ions in O-holes which causes the cubic close-packing of the oxygen atoms. Since the oxygen atoms are not very mobile only small grains are formed at first resulting in the diffuse diffraction patterns of the transition forms. At 870°C or above transformation to α-alumina takes place in the manner proposed by Ervin. Above 900°C, the x-ray diffraction lines become sharper because the oxygen atoms have greater mobility resulting in detectable grain growth.

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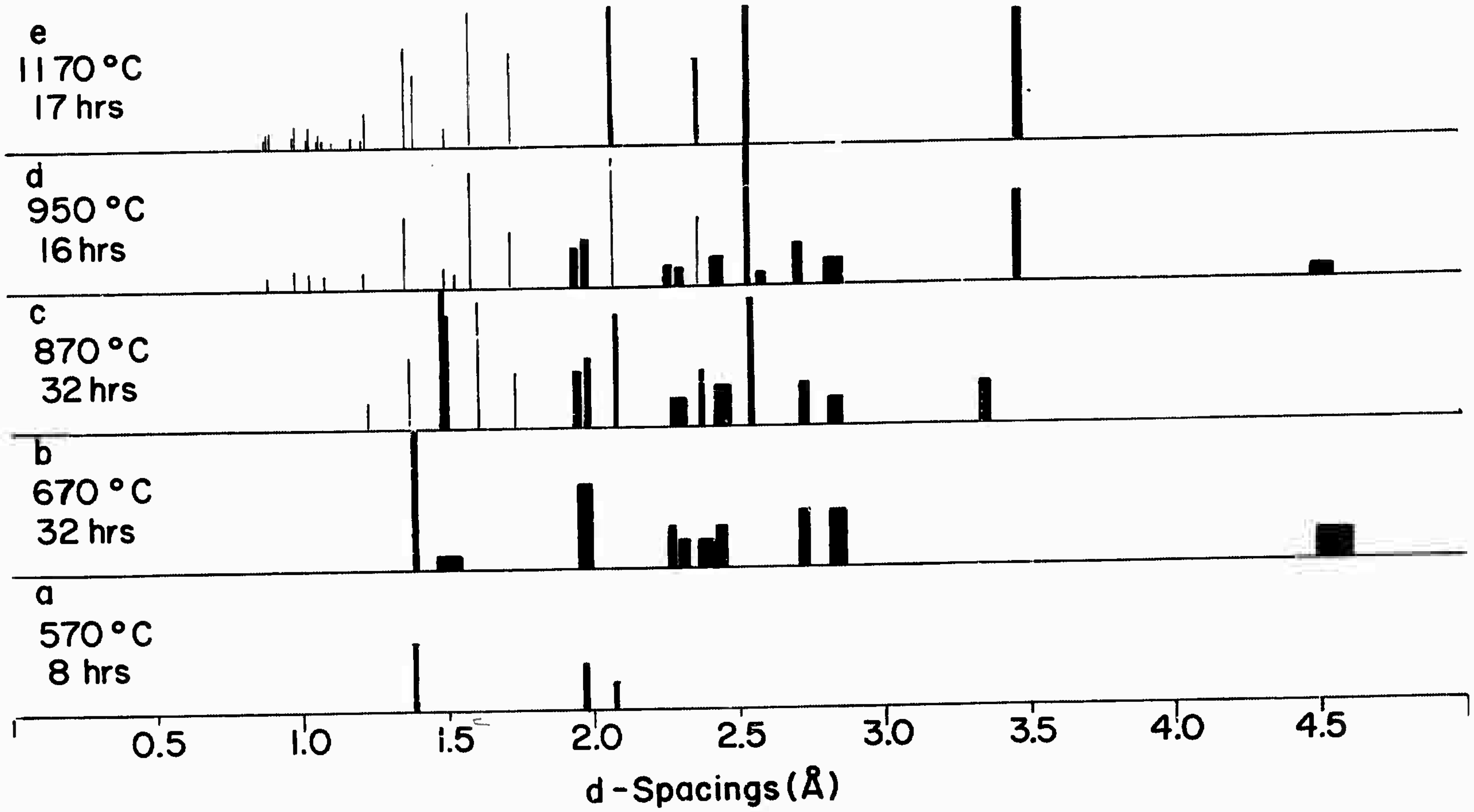


Figure 1. Transitions of Amorphous Al_2O_3 Films, d-spacings and Intensities

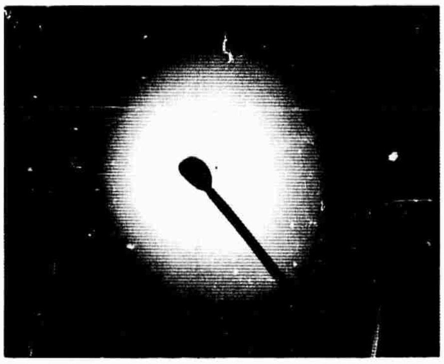
Figure 2. Electron Microscopic and Diffraction Study of Vapor-deposited Al_2O_3 Films

a. Edge of Film, No Heating, (28,000 X)

b. Feathering of Edge, 630°C, (11,000 X)

c. Film from Deposition on Glass, 620° to 630°C

d. Film from Deposition on Glass, 760°C



e. Film from Deposition on Sapphire, No Heating

Chapter 4

THE ENTHALPY OF GRAPHITE FROM 1200 to 2600°K

by E. D. West and S. Ishihara

Experimental

Under a related NBS project, measurements have been made of the increase in the enthalpy of graphite between the temperature of a calorimeter near room temperature and a furnace operating at temperatures from 1200 to 2600°K.

The specimen was a solid cylinder machined from a larger piece of grade CCH graphite (National Carbon Company) density 1.6 g/cm^3. According to the supplier, this grade is purified by the same treatment used for spectroscopic grades. After machining, it was heated in our furnace at temperatures up to 2700°K for several hours before measurements were begun. Spectrographic analysis showed less than 0.002% impurities.

The enthalpy data fit the equation

$$H_T-H_{298.15} = 28.9004T-1.045 \times 10^{-4}T^2-16126.2 \log_{10}T/313.15-8907.3$$

where H is in absolute Joules per gram atomic weight (12.01115) and T is in degrees Kelvin. The estimated standard error for an enthalpy value calculated from the equation does not exceed 0.14%. Systematic errors in measuring the furnace temperature are estimated to be not more than 0.3% due to the pyrometer calibration and not more than 0.4% due to the difference between the observed temperature and the average temperature of the capsule.

Enthalpy differences calculated from the equation agree with those reported by Evans [1] in Table 2-39 in a previous report (NBS No. 6645); differences range from a maximum of 1% below Table 2-39 at 1200°K to 0.7% above at 2500°K.

This work is to be presented along with a description of the method at the Third Symposium on Thermophysical Properties at Purdue University in March 1965.

Discussion

In the case of carbon, two questions must be considered in a presentation of the thermodynamic properties of the standard state: (1) are the data sufficiently accurate in themselves? (2) Do they refer to a standard crystalline form of carbon?

Enthalpy differences calculated from our equation lie consistently about 0.7% below the smooth data of McDonald [1] for spectroscopic grade SPK graphite (density 1.9). They agree with recent reviews of older data, maximum deviations being 1% below Dergazarian [3] et al. at 1200°K and 0.7% above Evans [1] at 2500°K. The heat capacity derived from our enthalpy equation are well within the scatter of the observations and the estimated accuracy of Rasor and McClelland [4] in the range 1500-2600°K. Since the older experimental work includes measurements on natural graphite, this consensus supports reasonable confidence that the enthalpy and heat capacity are known to a few percent from room temperature to 2600°K.

Regarding the second question, there is experimental evidence to indicate differences in the heat capacity of different graphites. DeSorbo [5] reports enthalpies at 298.15°K for Ceylon natural graphite and an Acheson graphite which differ by 88 J/gfw, almost twice the tolerance on the heat of formation of CO_2 set by Rossini and Jessup [6] in their paper recommending graphite as the standard state for carbon. The corresponding difference in heat capacity might be expected to extend at least to somewhat higher temperatures. There are obvious systematic trends amounting to several percent in the high temperature data for the four samples of Rasor and McClelland, but they state that these differences are not significant. The specific heat for pyrolytic graphite is reported to be from 10 to 50% above that of "ordinary" graphite in the temperature range 300 to 1300°K [7]. The difference in H_T-H_{298} between our measurements and those of McDonald on Al_2O_3 near 1200°K is about 0.3%. Taking this to represent the systematic difference between the two methods, we have 0.5% difference between smoothed values at 1200°K to ascribe to random errors of measurement or to a difference in the samples. Considering our standard error of 0.14% and a slightly larger value for McDonald's data, the 0.5% difference is too large to claim no significant difference in samples, but too small to be reasonably sure of a significant difference.

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Chapter 5

HIGH TEMPERATURE MATRIX SPECTROSCOPY

by D. E. Mann

1. MgF$_2$: Magnesium Fluoride: The infrared spectrum of MgF$_2$ isolated in a dilute solid krypton matrix at 20°K is presently being investigated in the apparatus described briefly below. Preliminary results in the region below 300 cm^{-1} have revealed a moderately intense band at 242 cm^{-1}*, as well as a few weak features at lower frequencies. The matrix was warmed from 20°K to 60°K and the 242 cm^{-1} band was found to decrease in intensity suggesting that it is monomeric rather than polymeric in origin. (Diffusion at the higher matrix temperatures would be expected to lead to increased band intensity if a di- or polymeric species was responsible for its occurrence.) Further experiments now in progress may provide corroboration of the assignment of the 242 cm^{-1} band to the ν_2 bending fundamental of MgF$_2$.

The apparatus now in use comprises (a) a variable-temperature cryostat which employs a Cryo-Tip liquefier unit; (b) an electron-bombardment furnace, and a Perkin-Elmer 301 far-infrared spectrometer.

2. Emission Spectrum of F$_2^+$: In the course of a recent investigation of the orange emission bands of F$_2$ (with Dr. T. L. Porter) a new band system was discovered which has now been assigned to the heretofore unrecorded species F$_2^+$. This is of special interest for the present program because F$_2^+$ is isoelectronic with the molecule FO. Twelve bands in the region 5300-4300 A have now been analyzed and have led to the conclusion that a portion of $A^2\pi$-$X^2\pi$ system of F$_2^+$ has been observed. It is expected that molecular constants for both states as well as estimates of their dissociation energies can be reported in the near future.

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*In agreement with Linevsky's results.

Chapter 6

HIGH TEMPERATURE, MASS SPECTROMETRIC STUDY OF THE COMPOUND, $Al_2O_3 \cdot BeO$

by J. Efimenko

I. The Al_2O_3-BeO System

A mass spectrometric study of this system is being made by observing the vapor species in equilibrium with selected, well characterized initial compositions as given in the solid-liquid phase diagram (Lang, Fillmore and Maxwell, J. Res. NBS 48, 301 (1952)).

Experimental

The $Al_2O_3 \cdot BeO$ compound was synthesized from alumina, having a carbon content below 0.0034, and beryllia by fusion in an arc image hot spot by A. Dragoo at NBS. During the preparation the fused material did not come into contact with any metallic container. The solid was crushed in a diamond mortar and ground in an alumina mortar. A sample of the material was placed in a tungsten cup and inserted into a tungsten effusion cell. Temperature-intensity data were collected for the species: Be^+, O^+, Al^+, O_2^+, $AlOBe^+$, Al_2O^+ and $(BeO)_2^+$ in the temperature range 2180°-2570°K.

Discussion

The reactions selected for consideration are the following:

(1) $Al(g) + Be(g) + O(g) \rightleftarrows AlOBe(g)$

(2) $2Al(g) + O(g) \rightleftarrows Al_2O(g)$

(3) $Al_2O(g) + Be(g) \rightleftarrows AlOBe(g) + Al(g)$

(4) $1/2\ O_2(g) \rightleftarrows O(g)$

(5) $Al_2O_3 \cdot BeO(l) \rightleftarrows 2Al(g) + Be(g) + 4\,O(g)$

Table 1 contains the partial pressures in atmospheres of the species considered.

Table 1

Mass Spectrometric Temperature-Partial Pressure Data

T °K	Atmospheres					
	P_{Be}	P_O	P_{Al}	P_{AlOBe}	P_{Al_2O}	P_{O_2}
	$x10^{-7}$	$x10^{-7}$	$x10^{-8}$	$x10^{-10}$	$x10^{-10}$	$x10^{-8}$
2152	0.225	0.360	0.840	0.0152	0.207	
2211	0.513	0.914	2.09	0.162	0.593	
2290	1.27	2.15	6.26	0.700	2.27	
2179	0.275	0.394	0.980	0.0523	2.15	
2226	0.480	0.800	1.37	0.151	0.54	
2279	0.931	1.61	0.435	0.468	1.35	
2337	1.88	3.43	10.10	1.280	3.95	
2205	0.397	0.654	1.[illegible]	0.0952	0.0426	
2290	1.12	1.96	5.30	0.592	1.94	
2290	1.11	1.88	5.30	0.592	1.88	
2343	2.14	3.90	11.60	1.57	4.73	
2417	4.77	9.00	29.70	4.27	12.60	1.05
2470	8.20	16.70	53.50	8.26	24.80	1.84
2518	1.17	29.20	95.00	17.00	49.00	3.57
2567	17.80	42.40	135.00	19.30	50.80	4.35

These partial pressures were computed from the relation, $p = \frac{I^+T}{S\sigma\gamma}$, where S is the instrument sensitivity for each specie; σ, relative ionization cross-section; γ, the multiplier efficiency for each specie; I^+, the ion intensity. The instrument sensitivity for silver, the calibrating material, was converted to specie sensitivity by the relation:

$$S_x = S_{Ag} \cdot \frac{\sigma_x}{\sigma_{Ag}} \cdot \frac{T_{Ag}}{T_x} \cdot \frac{\gamma_x}{\gamma_{Ag}}$$

Table 2 lists auxiliary computation data.

Table 2

Auxiliary Computation Data

Specie	Sensitivity Values $\sigma_{(1)}$	$\gamma_{(2)}$	T °K
Ag	34.8	2000	1275
Be	6.3	2800	
O	3.3	4200	
Al	15.4	2500	
O_2	6.6	5000	
AlOBe	25.0	5000	
Al_2O	34.1	5000	

Note: (1) J. W. Otvos and D. P. Stevenson, J. Am. Chem. Soc. 78, 546-551 (1956)

(2) Average values obtained experimentally by the author

(3) Silver sensitivity SAg = 5.0×10^{-7} amp/mm Hg

Free Energy Functions

Be	Table A-4, NBS Report 6928, July, 1960
O	Table A-8, NBS Report 6928, July, 1960
Al	Table A-13, NBS Report 6928, July 1960
O_2	Table A-83, NBS Report 7437, January, 1962
Al_2O	Table A-57, NBS Report 8186, January, 1964
AlOBe	Table A-90, NBS Report 8504, July, 1964

With the aid of free energy functions and equilibrium constants for the reaction (1)-(4), the enthalpies change at absolute zero were computed and listed in Table 3.

Table 3

Enthalpy Changes from Free Energy Functions

Reaction	(1)	(2)	(3)	(4)
T °K	$-\Delta H_0^\circ$ kcal/mol	$-\Delta H_0^\circ$ kcal/mol	$+\Delta H_0^\circ$ kcal/mol	$+\Delta H_0^\circ$ kcal/mol
2152	223.14	260.65	37.51	
2211	228.11	248.05	19.94	
2290	230.51	249.36	18.85	
2179	229.30	260.39	31.09	
2226	232.26	253.79	17.10	
2279	231.71	250.51	18.80	
2337	231.64	263.22	31.58	
2205	229.25	250.38	21.63	
2290	231.15	250.34	19.19	
2290	231.16	250.69	19.53	
2343	231.32	251.00	19.68	
2417	235.92	250.16	14.24	59.29
2470	235.96	251.00	15.04	59.92
2518	247.72*	250.01	2.29*	60.23
2567	235.91	250.38	14.47	57.67
	<231.24>	<253.10>	<21.30>	<59.28>

Note (1) < > , the arithmetic mean value

(2) * enthalpy not included in mean value.

Experimental data permitted graphical derivation of the ΔH values also and a summary is presented in Table 3A.

Table 3A

Enthalpies Changes-Summary

Method	van't Hoff Equation		Free Energy Functions
Reactive	$\Delta H^\circ_{<2350>}$ kcal/mol	ΔH°_0 kcal/mol	ΔH°_0 kcal/mol
(1)	-228.0	-221.8	-231.2 ± 3.3
(2)	-275.0	-269.5	-253.1 ± 4.6
(3)	+ 24.8	+ 25.5	+ 21.3 ± 6.2
(4)			+ 59.3 ± 1.0
(5)	+826.0		

Note: (a) The error shown is the mean square deviation

Reactions (2) and (4) permit a check on the reliability of the data since both reactions have been already studied. The enthalpy for dissociation of O_2 (g) is 58.983 kcal/mol (NBS Report 8504, p. 165, July, 1964)) and the value from this study is $\Delta H^\circ_0 = 59.28$. The enthalpy change for reaction (2), $\Delta H^\circ_0 = -253.1$ kcal/mol, is within experimental error of other reported values, -254 ± 7 kcal/mol (R. F. Porter, P. Schissel and M. G. Inghram, J. Chem. Phys. 23, 399 (1955)) and -243.4 ± 7 (J. Drowart, G. De Maria, R. P. Burns and M. G. Inghram, J. Chem. Phys. 32, 1372 (1960)). These comparisons indicate that the present data may be somewhat high.

For reaction (5) the enthalpy change could be obtained only by use of the van't Hoff relation since free energy functions are lacking for $Al_2O_3 \cdot BeO$ liquid in the experimental range of temperatures.

Various sources of errors must be considered in the experimental data. At the conclusion of some runs, it was observed that the initial orifice area was decreased by a deposit of crystals about the perimeter. Under the microscope they had a metallic appearance and very likely were tungsten. The effect occurred in spite of the fact that the orifice half of the cells appeared approximately 50° hotter than the bottom half of the effusion cell. The magnitude of error this effect caused is uncertain but assumed to be small or negligible since the sampling area of the beam was less than the orifice image area. Experimentally the beam intensity was noticed not to decrease until the orifice closed to a very small size.

An analysis of systematic errors will not be made at the present time since one assumes that they remain constant throughout an experiment. Evidence is being accummulated on the effect of temperature, ion-intensity, multiplier efficiency and instrument sensitivity.

For the enthalpy changes for reactions (1), (2), (3) and (4) ar computed the Mean-Square Deviations, σ.

$$\sigma = \left(\frac{\Sigma d^2}{n} \right)^{1/2}, \text{ where } d = Xn-\bar{X} \text{ and } \bar{X} \text{ is the}$$

arithmetic mean.

Preliminary measurements were made on the $3Al_2O_3\cdot BeO$ compound in the temperature range 1800°-2100°C (uncorrected). The mass spectrometric peaks detected correspond to the following ions: Be^+, O^+, Al^+, AlO^+, Al_2O^+ plus alkali and alkaline earth impurities. An arc image sample of the 3:1 mol ratio compound has been prepared and will be examined at high temperatures.

APPENDIX I

FORMULA-PROPERTY INDEX FOR THE FIRST TWELVE PRELIMINARY REPORTS

by Howard W. Flieger, Jr.

An index has been prepared for the first twelve Preliminary Reports to assist the reader in searching for the properties of materials in his interest. The present (13th) report is excluded in this index.

For the purpose of this index the NBS report numbers are referred to as the following Volume numbers:

NBS REPORT	VOLUME NUMBER
6297	1
6484	2
6645	3
6928	4
7093	5
7192	6
7437	7
7587	8
7796	9
8033	10
8186	11
8504	12

The arrangement of the chemical formulae in the index is alphabetical. The placement of the chemical symbols within a given formula is also alphabetical. Chemical isomers are not distinguished. In general four printing spaces are allocated to a chemical symbol and its numerical occurrence in a fromula. For example, lithium aluminum fluoride, Li_3AlF_6, will be found in the index as AL F 6LI 3. The components of chemical systems are separated by a series of hyphens. Thus Al_2O_3-TiO_2 appears as AL 20 3----O 2TI. In future versions of the index the spacing may be condensed and the numbers may appear as subscripts.

The property and/or study reference consists of two parts; a letter followed by a number. The letter indicates the property or study and the number indicates the source or treatment of the information. The interpretation of the letters and numbers is found in the Key below.

The location of the references in the reports appaears as the Volume number above followed by the page number in parentheses. An exception to this rule occurs for Volumes 2, 3 and 4 where the pages in the appendices have not been numbered. For reference to be found in these appendices the Table number appears within the parentheses.

The extensive bibliographies found in several of the Preliminary Reports have not been included in the index. These bibliographies are listed below.

TITLE	VOLUME	PAGES
A Brief Review of the Heat Relationships Among the Crystalline Oxides and Oxyhydrates of Aluminum.	1	74-85
References to Recent Values for Heats of Formation.	5	169-173
The Heats of Formation of Inorganic Fluorine Compounds--A Survey.	6	92-175
Recent Additions to the Literature on the Chemistry of the Light Elements.	7	39-60
Thermochemical Data for Some Simple Hydrides and Inorganic Oxidizers.	7	79-89
Recent Additions to the Literature Related to the Heats of Formation of Compounds of Selected Elements.	8	76-89
New Literature Relating to Heats of Formation of the Light Elements and Their Compounds.	9	40-81
Substance-Property Index for 1962.	9	82-156
A Bibliography Relating to Heats of Formation, Enthalpy Changes Resulting from Phase Changes, and the Heat Capacities of Aluminum and Beryllium Fluorides, Oxyfluorides, Chlorides, and Oxychlorides, and of Lithium Fluoride.	10	22-35
New Literature Relating to Heats of Formation of Fluorine Compounds of Selected Elements.	11	122-142
Preliminary List of Ionization Potentials or Electron Affinities of Light Element Compounds.	12	185-202

KEY to property or study:

Property or Study Letter	Interpretation
A	Heats of reaction, dissociation and formation.
B	Thermodynamic functions of solids, liquids and solutions.
C	Thermodynamic functions of gases.
D	Vapor pressure and vaporization equilibria, decomposition and dissociation studies, and heats of vaporization and sublimation.
E	Data of state and related physical properties.
F	Phase diagrams.
G	Absorption and emission spectroscopy including molecular constants.
H	Kinetic studies.
J	Chemical preparation and/or purification studies.
K	Electrical discharge (exploding wire) studies.
L	Calorimetry techniques.
M	Mass spectroscopy studies.

Source and Treatment Number	Source and/or treatment of information
1	NBS reported.
2	Literature (non-NBS) reported.
3	NBS critical evaluation, review and analysis of data.
4	Non-NBS critical evaluation, review and analysis of data.
5	Tables at a standard state.
6	Ideal Gas tables.
7	Theoretical or empirical estimate.
8	Apparatus description.
9	Tables of thermodynamic properties with temperature or pressure argument and other tables.

FORMULA-PROPERTY INDEX FOR THE FIRST TWELVE PRELIMINARY REPORTS

FORMULA	PROPERTY OR STUDY	VOLUME AND PAGE
AG	C5	12(184)
AG CL	C5	12(184)
AG 2O	C5	12(184)
AG+	C5	12(184)
AL	A2	1(58)
AL	A2	2(101)
AL	A5	4(C 1)
AL	B2	1(7)
AL	B2	2(22)
AL	B3	1(26)
AL	B5	1(9)
AL	B5	2(20)
AL	B9	2(2- 1)
AL	B9	4(B 1)
AL	C6	2(1-13)
AL	C6	4(A13)
AL	D2	1(48)
AL	K1	12(26)
AL+	C6	6(229)
AL--B	F2	5(187)
AL B 3H 12	A2	7(92)
AL B 10	F2	5(150)
AL B 12	F2	5(150)
AL--BF	F2	5(188)
AL BF O	C6	12(140)
AL BF O	G7	12(85)
AL BR 3	B7	6(54)
AL C	A2	3(2)
AL C	A2	3(65)
AL C	A5	4(C 2)
AL C	G2	4(43)
AL CL	A2	1(59)
AL CL	A2	1(66)
AL CL	A2	2(89)
AL CL	A2	2(102)
AL CL	A5	4(C 2)
AL CL	C6	1(125)
AL CL	C6	2(1-30)
AL CL	C6	4(A32)
AL CL	D3	8(114)
AL CL	G1	12(57)
AL CL	G2	1(42)
AL CL	G2	4(43)
AL CL	G6	12(64)
AL CL	G6	12(65)
AL CL	G6	12(66)
AL CL	G9	2(50)
AL CL F 2	C6	2(1-61)
AL CL F 2	C6	4(A65)
AL CL F 2	G2	1(44)
AL CL F 2	G9	2(51)
AL CL O	B5	1(9)
AL CL O	C6	2(1-58)
AL CL O	C6	4(A62)
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AL CL O	G9	2(51)
AL CL 2	A2	1(59)
AL CL 2	A2	2(89)
AL CL 2	A2	2(102)
AL CL 2	A5	4(C 2)
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AL CL 2	G9	2(51)
AL CL 2F	C6	2(1-62)
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AL CL 2F	G2	1(44)
AL CL 2F	G9	2(51)
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AL CL 3	A2	1(66)
AL CL 3	A2	2(89)
AL CL 3	A2	2(103)
AL CL 3	A3	4(36)
AL CL 3	A5	4(C 2)
AL CL 3	B2	3(64)
AL CL 3	B3	1(26)
AL CL 3	B5	1(9)
AL CL 3	B5	2(20)
AL CL 3	B	2(2- 6)
CL N O	C5	12(178)
CL N O 2	A2	7(94)
CL N O 2	C5	12(178)
CL N O 5	A2	7(94)
CL N O 5	B5	12(178)
CL N O 6	A2	7(94)
CL N O 6	B5	12(178)
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CL NA	B2	9(21)
CL NA	B2	11(90)
CL NA	B3	11(90)
CL NA	B9	9(31)
CL NA	B9	11(167)
CL NA	G9	10(19)
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CL O	A2	7(94)
CL O	C5	12(167)
CL O	C6	1(135)
CL O	C6	2(1-35)
CL O	C6	4(A38)
CL O	G2	1(42)
CL O	G9	2(50)
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CL O 2	A2	7(94)
CL O 2	B5	12(167)
CL O 2-	B5	12(167)
CL O 3	C5	12(167)
CL O 3-	B5	12(167)
CL O 4-	B5	12(167)
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CL O 6N	A8	7(3)
CL O 6N	A9	7(9)
CL O 6N	B1	7(3)
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CL 2	A2	2(101)
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CL 2	A7	2(41)
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CL 2	C5	12(167)
CL 2	C6	1(131)
CL 2	C6	2(1-33)
CL 2	C6	4(A36)
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CL 2	G9	2(50)
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CL 2CR	B2	12(92)
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CL 2H 2MG O	B2	2(27)
CL 2H 2MG O	B5	1(17)
CL 2H 2MG O	B5	2(20)
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CL 2H 2MG O	B9	4(B16)
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CL 2H 4MG O 2	A2	2(104)
CL 2H 4MG O 2	A5	4(C 2)
CL 2H 4MG O 2	B2	1(15)
CL 2H 4MG O 2	B2	2(27)
CL 2H 4MG O 2	B5	1(17)
CL 2H 4MG O 2	B5	2(20)
CL 2H 4MG O 2	B9	4(B17)
CL 2H 4MG O 4	B9	2(2-17)
CL 2H 6N 2	B5	12(178)
CL 2H 8MG O 4	A2	2(96)
CL 2H 8MG O 4	A2	2(104)
CL 2H 8MG O 4	A5	4(C 2)
CL 2H 8MG O 4	B2	1(15)
CL 2H 8MG O 4	B2	2(27)
CL 2H 8MG O 4	B5	1(17)
CL 2H 8MG O 4	B5	2(20)
CL 2H 8MG O 4	B9	2(2-18)
CL 2H 8MG O 4	B9	4(B18)
CL 2H 12MG O 6	A2	2(96)
CL 2H 12MG O 6	A2	2(104)
CL 2H 12MG O 6	A5	4(C 2)

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AL CL 3	C6	2(1-64)
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AL CL 3	S2	4(36)
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AL CL 3H 120 6	A2	2(103)
AL CL 3H 120 6	A5	4(C 2)
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AL F	A2	1(65)
AL F	A2	2(88)
AL F	A2	2(102)
AL F	A2	3(65)
AL F	A5	4(C 2)
AL F	C6	1(123)
AL F	C6	2(1-29)
AL F	C6	4(A31)
AL F	D3	8(114)
AL F	G1	9(12)
AL F	G1	12(57)
AL F	G2	1(42)
AL F	G2	4(43)
AL F	G6	12(64)
AL F	G6	12(65)
AL F	G9	2(50)
AL F	G9	4(47)
AL F	G9	9(14)
AL F O	B5	1(9)
AL F O	C6	2(1-57)
AL F O	C6	4(A61)
AL F O	G2	1(44)
AL F O	G9	2(51)
AL F 2	A2	1(59)
AL F 2	A2	1(66)
AL F 2	A2	2(88)
AL F 2	A2	2(102)
AL F 2	C6	2(1-59)
AL F 2	C6	4(A63)
AL F 2	G2	1(44)
AL F 2	G9	2(51)
AL F 3	A1	8(13)
AL F 3	A1	12(21)
AL F	A2	1(59)
AL F 3	A2	1(66)
AL F 3	A2	2(88)
AL F 3	A2	2(102)
AL F 3	A2	3(65)
AL F 3	A2	4(35)
AL F 3	A2	8(13)
AL F 3	A5	4(C 2)
AL F 3	B2	2(24)
AL F 3	B3	1(26)
AL F 3	B5	1(9)
AL F 3	B5	2(20)
AL F 3	B9	2(2- 5)
AL F 3	B9	4(B 5)
AL F 3	C6	2(1-60)
AL F 3	C6	4(A64)
AL F 3	D1	9(156)
AL F 3	D3	2(68)
AL F 3	D8	9(158)
AL F 3	D9	9(164)
AL F 3	D9	9(165)
AL F 3	G2	1(44)
AL F 3	G9	2(51)
AL F 3	L1	8(13)
ALF3-AL203-FLI	F2	5(156)
ALF3--AL203--FLI	F2	5(206)
AL F 3----F K	F2	5(222)
AL F 3----F L+	F2	5(155)
AL F 3----F L)	F2	5(165)
AL F 3----F LI	F2	5(220)
AL F 3----F NA	F2	5(221)
AL F 3H 60 3	A2	1(59)
AL F 6LI O	B9	11(74)
AL F 6L) 3	B1	11(68)
AL F 6LI 3	B9	11(71)
AL F 6LI 3	B9	11(162)
AL F 6NA 3	B2	9(20)
CL 2H 12MG O 6	B2	1(16)
CL 2H 12MG O 6	B2	2(28)
CL 2H 12MG O 6	B5	1(17)
CL 2H 12MG O 6	B5	2(20)
CL 2H 12MG O 6	B9	2(2-19)
CL 2H 12MG O 6	B9	4(B19)
CL 2LI 2	A2	1(61)
CL 2L) 2	A2	1(72)
CL 2LI 2	A2	2(99)
CL 2L(2	A2	2(105)
CL 2L) 2	A5	4(C 2)
CL 2L1 2	C6	2(1-46)
CL 2LI 2	C6	4(A50)
CL 2LI 2	G2	1(43)
CL 2L) 2	G9	2(51)
CL 2MG	A2	2(95)
CL 2MG	A2	2(104)
CL 2MG	A5	4(C 2)
CL 2MG	B2	1(15)
CL 2MG	B2	2(26)
CL 2MG	B3	1(26)
CL 2MG	B5	1(17)
CL 2MG	B5	2(20)
CL 2MG	B9	2(2-15)
CL 2MG	B9	4(B15)
CL 2MG	C6	2(1-51)
CL 2MG	C6	4(A55)
CL 2MG	D3	2(73)
CL 2MG	G2	1(43)
CL 2MG	G9	2(51)
CL 20	A2	7(94)
CL 20	C5	12(167)
CL 20 S	B5	12(173)
CL 20 S	C5	12(173)
CL 20 2S	B5	12(174)
CL 20 2S	C5	12(174)
CL 20 5S 2	B5	12(174)
CL 20 5S 2	C5	12(174)
CL 20 7	A2	7(94)
CL 20 7	C5	12(167)
CL 2PB	B2	6(53)
CL 2PB	B3	6(53)
CL 2PB	C5	12(184)
CL 2S 2	B5	12(173)
CL 2S 2	C5	12(173)
CL 2SE 2	B5	12(174)
CL 2SE 2	C5	12(174)
CL 3CR	B2	12(92)
CL 3FF	B2	12(96)
CL 31	A2	7(94)
CL 3I	B5	12(171)
CL 3LI 3	A2	1(61)
CL 3L) 3	A2	2(99)
CL 3LI 3	A2	2(105)
CL 3LI 3	A5	4(C 2)
CL 3N	A2	7(94)
CL 3N	B5	12(178)
CL 30 P	B5	12(182)
CL 30 P	C5	12(182)
CL 3P	B5	12(182)
CL 3P	C5	12(182)
CL 3P S	C5	12(182)
CL 3P +	C5	12(182)
CL 4TE	B5	12(175)
CL 4ZR	B2	5(179)
CL 4ZR	B9	5(252)
CL 5P	B5	12(182)
CL 5P	C5	12(182)
CR	B2	12(91)
CR K 20 4	B2	12(98)
CR 2FF O 4	B2	12(96)
CR 2K 20 7	B2	12(98)
CR 20 3	B2	12(92)
CS)	G9	10(19)
O	C5	12(165)
O F 2N	C)	8(125)
D F 2N	C6	8(130)
O F 2N	G1	8(125)
O H O	B5	12(165)
O H O	C5	12(165)

AL F 6NA 3	B9	9(31)
AL H	A2	1(59)
AL H	A2	2(86)
AL H	A2	2(102)
AL H	A5	4(C 2)
AL H	A7	2(41)
AL H	C6	4(A30)
AL H	G2	4(43)
AL H	G9	4(47)
AL H	J2	1(99)
AL H O	C6	2(1-55)
AL H O	C6	4(A59)
AL H O	G2	1(44)
AL H O	G2	1(44)
AL H O	G9	2(51)
AL H O	G9	2(51)
AL H O 2	C5	2(1-56)
AL H O 2	C6	4(A60)
AL H 3	A2	1(59)
AL H 3	A2	1(65)
AL H 3	A2	2(87)
AL H 3	A2	2(102)
AL H 3	A5	4(C 2)
AL H 3	B5	1(9)
AL H 3ME 6N 4	A9	3(59)
AL H O 2	G2	1(44)
AL H O 2	G9	2U 8D
AL H 3ME 6N 4	D9	3(57)
AL H 3ME 6N 4	D9	3(59)
AL H 3O 3	A2	1(59)
AL H 3O 3	A2	1(65)
AL H 3O 3	A2	2(88)
AL H 3O 3	A2	2(102)
AL H 3O 3	A5	4(C 2)
AL H 4LI	A2	7(92)
AL H 4LI	B2	1(21)
AL H 4LI	B5	1(22)
AL I 3	B7	6(54)
AL K O 4SI	B2	12(97)
AL K O 6SI	B2	12(97)
AL K O 8SI 3	B2	12(97)
AL K O 8SI 3	B2	12(98)
AL--LI	F2	5(189)
AL LI O 2	B2	1(21)
AL LI O 2	B2	2(30)
AL LI O 2	B5	1(22)
AL LI O 2	B5	2(20)
AL LI O 2	B9	2(2-27)
AL LI O 2	B9	4(B27)
AL--MG	F2	5(190)
AL N	A2	2(90)
AL N	A2	2(103)
AL N	A2	3(2)
AL N	A2	3(65)
AL N	A2	4(35)
AL N	A2	4(36)
AL N	A3	4(36)
AL N	A5	4(C 2)
AL N	B2	3(14)
AL N	B3	3(14)
AL N	B5	3(16)
AL N	B5	3(21)
AL N	B9	3(22)
AL N	B9	3(2-31)
AL N	B9	4(B31)
AL N	D9	3(38)
AL N	J2	4(26)
AL NA C 2	B9	9(31)
AL O	A2	1(59)
AL O	A2	1(62)
AL O	A2	2(83)
AL O	A2	2(102)
AL O	A5	4(C 2)
AL O	C6	1(127)
AL O	C6	2(1-28)
AL O	C6	4(A29)
AL O	G2	1(42)
AL O	G2	4(45)
AL O	G9	2(50)
AL--O	D2	1(50)
D O	C5	12(165)
D 2	C5	12(165)
D 20	B5	12(165)
D 20	C5	12(165)
E -	C6	7(109)
F	A2	1(58)
F	A2	2(101)
F	A5	4(C 1)
F	C5	12(166)
F	C6	2(1- 9)
F	C6	4(A 9)
F +	C5	12(166)
F +	C6	6(221)
F -	B5	12(166)
F -	C5	12(166)
F -	C6	12(128)
F CS	G9	10(19)
F H	A2	7(90)
F H	B5	12(166)
F H	C5	12(166)
F H	C6	2(1-32)
F H	C6	4(A35)
F H	G1	4(46)
F H	G2	4(46)
F H	G9	4(47)
F H 4N	B2	9(27)
F H 4N	B3	10(40)
F H 4N	B5	12(178)
F H 4N	B9	9(32)
F H 4N	B9	10(79)
F H 6N O	B2	9(28)
F H 6N O	B3	10(40)
F H 6N O	B5	12(178)
F H 6N O	B9	9(32)
F H 6N O	B9	10(80)
F K	B2	7(70)
F K	B2	11(90)
F K	B3	11(90)
F K	B9	11(171)
F K	G9	10(19)
F LI	A2	1(61)
F LI	A2	1(71)
F LI	A2	2(97)
F LI	A2	2(98)
F LI	A2	2(105)
F LI	A2	12(23)
F LI	A5	4(C 2)
F LI	B1	1(20)
F LI	B2	1(20)
F LI	B2	2(29)
F LI	B2	2(29)
F LI	B3	1(27)
F LI	B5	1(22)
F LI	B5	1(33)
F LI	B5	2(20)
F LI	B9	2(2-25)
F LI	B9	4(B24)
F LI	C6	1(107)
F LI	C6	2(1-20)
F LI	C6	4(A20)
F LI	D2	4(36)
F LI	D3	2(74)
F LI	D3	2(77)
F LI	G2	1(42)
F LI	G9	2(50)
F LI	G9	10(19)
F LI--F 2MG	F2	5(164)
F LI--F 2MG	F2	5(219)
F LI--F 4ZR	F2	5(166)
F LI--F 4ZR	F2	5(223)
F MG	A2	1(60)
F MG	A2	1(70)
F MG	A2	2(95)
F MG	A2	2(104)
F MG	A5	4(C 2)
F MG	C6	1(117)
F MG	C6	2(1-26)
F MG	C6	4(A26)
F MG	G2	1(42)
F MG	G9	2(50)

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AL--O                 D2      2( 61)   |  F   N    O         C5    12(178)
AL--O                 H1      8( 55)   |  F   N    O   2     C5    12(178)
AL--O                 M8      8( 56)   |  F   N    S         B5    12(180)
AL  O    BE+          M1     12(118)   |  F   NA             B2     9( 20)
AL  O  2              A2      1( 59)   |  F   NA             B2    11( 89)
AL  O  2-             A2      1( 63)   |  F   NA             B3    11( 89)
AL  O  2-             A2      2( 84)   |  F   NA             B9     9( 31)
AL  O  2-             A2      2(102)   |  F   NA             B9    11(165)
AL  O  2-             A5      4(C 2)   |  F   NA             G9    10( 19)
AL  O  2NA            B2      9( 20)   |  F   O              C5    12(166)
AL  S                 C6      4(A33)   |  F   RB             G9    10( 19)
AL  S                 G2      4( 45)   |  F  2               A2     1( 58)
AL  S                 G9      4( 47)   |  F  2               A2     2(101)
AL--SI                F2      5(191)   |  F  2               A5     4(C 1)
AL--TI                F2      5(192)   |  F  2               A7     2( 41)
AL--ZR                F2      5(193)   |  F  2               C5    12(166)
AL 2                  A2      1( 59)   |  F  2               C6     1(129)
AL 2                  A2      1( 62)   |  F  2               C6     2(1-31)
AL 2                  A2      2( 83)   |  F  2               C6     4(A34)
AL 2                  A2      2(102)   |  F  2               G2     1( 42)
AL 2                  A5      4(C 2)   |  F  2               G9     2( 50)
AL 2                  A7      2( 41)   |  F  2+              C5    12(166)
AL 2                  G2      4( 42)   |  F  2FE             B2    12( 96)
AL 2                  C6      4(A28)   |  F  2H    K         B2     7( 70)
AL 2                  G9      4( 47)   |  F  2H    LI        A2     2( 99)
AL 2BA  0  4          A2      6( 83)   |  F  2H    LI        A2     2(105)
AL 2BA  0  4          A3      6( 83)   |  F  2H    LI        A5     4(C 2)
AL 2BA 30  4          A2      6( 83)   |  F  2H    LI        B2     9( 15)
AL 2BA 30  4          A3      6( 83)   |  F  2H    LI        B9     9( 31)
AL 2BE  0  4          A2      6( 83)   |  F  2H    N         C1     8(125)
AL 2BE  0  4          A3      6( 83)   |  F  2H    N         C5    12(178)
AL 2BE  0  4          B1      8( 44)   |  F  2H    N         C6     8(128)
AL 2BE  0  4          B1     11( 50)   |  F  2H    N         G1     8(125)
AL 2BF  0  4          B1     11( 62)   |  F  2H    NA        B2     9( 20)
AL 2BF  0  4          B2      8( 50)   |  F  2H    NA        B3    10( 40)
AL 2BE  0  4          B9      8( 49)   |  F  2H    NA        B9     9( 31)
AL 2BE  0  4          B9      8( 52)   |  F  2H    NA        B9    10( 69)
AL 2BE  0  4          B9      8(172)   |  F  2H -            B5    12(167)
AL 2BE  0  4          B9     11( 58)   |  F  2LI 2           A2     1( 61)
AL 2BE  0  4          B9     11( 64)   |  F  2LI 2           A2     1( 71)
AL 2BE  0  4          B9     11(160)   |  F  2LI 2           A2     2( 98)
AL 2BE  0  4          E2      5(160)   |  F  2LI 2           A2     2(105)
AL 2BE  0  4          J1     12( 83)   |  F  2LI 2           A5     4(C 2)
AL 2C  2              A2      2( 90)   |  E  2LI  2          C6     2(1-45)
AL 2C  2              A2      2(103)   |  F  2LI 2           C6     4(A49)
AL 2C  2              A2      3(  3)   |  F  2LI 2           G2     1( 43)
AL 2C  2              A2      3( 65)   |  F  2LI 2           G9     2( 51)
AL 2C  2              A5      4(C 2)   |  F  2MG             A2     1( 60)
AL 2CA  0  4          A2      6( 83)   |  F  2MG             A2     2( 95)
AL 2CA  0  4          A3      6( 83)   |  E  2MG             A2     2(104)
AL 2CA  0  4          B2     12( 89)   |  F  2MG             A2     4( 38)
AL 2CA  0  8SI 2      B2     12( 89)   |  F  2MG             A2    12( 22)
AL 2CA 20  7SI        B2     12( 89)   |  F  2MG             A3     4( 38)
AL 2CA 30  4          A2      6( 83)   |  F  2MG             A5     4(C 2)
AL 2CA 30  4          A3      6( 83)   |  F  2MG             B2     1( 15)
AL 2CA 30  6          B2     12( 89)   |  F  2MG             B2     2( 26)
AL 2CL 6              A2      1( 59)   |  F  2MG             B3     1( 26)
AL 2CL 6              A2      1( 66)   |  F  2MG             B5     1( 17)
AL 2CL 6              A2      1( 67)   |  F  2MG             B5     2( 20)
AL 2CL 6              A2      2( 90)   |  F  2MG             B9     2(2-14)
AL 2CL 6              A2      2(103)   |  F  2MG             B9     4(B14)
AL 2CL 6              A2      4( 36)   |  F  2MG             C6     2(1-50)
AL 2CL 6              A3      4( 36)   |  F  2MG             C6     4(A54)
AL 2CL 6              A5      4(C 2)   |  F  2MG             O3     2( 71)
AL 2CL 6              A5      4(C 2)   |  F  2MG             D3     2( 72)
AL 2CL 6              C6      2(1-65)  |  F  2MG             G2     1( 43)
AL 2CL 6              C6      4(A69)   |  F  2MG             G9     2( 51)
AL 2F  6              D3      2( 70)   |  F  2N              C5    12(178)
AL 2FE  0  4          B2     12( 96)   |  F  2N              C6     6(241)
AL 2H  20  4          A2      1( 59)   |  F  2N              G1     6( 33)
AL 2H  20  4          A2      1( 64)   |  F  2N              G2     6( 33)
AL 2H  20  4          A2      2( 86)   |  F  2N  2           C5    12(178)
AL 2H  20  4          A2      2(102)   |  F  20              C5    12(166)
AL 2H  20  4          A5      4(C 2)   |  F  20    S         C5    12(173)
AL 2H  20  4          B2      1(  7)   |  F  20  2           C5    12(166)
AL 2H  20  4          B2      2( 23)   |  F  20  2S          C5    12(173)
AL 2H  20  4          B5      1(  9)   |  F  20  3           C5    12(166)
AL 2H  20  4          B5      2( 20)   |  F  2PB             B7     6( 53)
AL 2H  20  4          B9      2(2- 3)  |  F    3CR           B2    12( 92)
AL 2H  20  4          B9      4(B 3)   |  F  3LI 3           A2     1( 61)
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AL 2H  20  4     E2    1( 88)
AL 2H  20  4     J2    1( 90)
AL 2H  20  4     J2    1( 91)
AL 2H  20  4     B3    1( 26)
AL 2H  60  6     A2    1( 59)
AL 2H  60  6     A2    1( 64)
AL 2H  60  6     A2    1( 65)
AL 2H  60  6     A2    2( 86)
AL 2H  60  6     A2    2(102)
AL 2H  60  6     A5    4(C 2)
AL 2H  60  6     B2    1(  8)
AL 2H  60  6     B2    2( 23)
AL 2H  60  6     B3    1( 26)
AL 2H  60  6     B5    1(  9)
AL 2H  60  6     B5    2( 20)
AL 2H  6-  6     B9    2(2- 4)
AL 2H  60  6     B9    4(B 4)
AL 2H  60  6     E2    1( 88)
AL 2H  60  6     J2    1( 90)
AL 2LI 20  4     A2    6( 83)
AL 2LI 20  4     A3    6( 83)
AL 2MG  0  4     B2    1( 16)
AL 2MG  0  4     B2    2( 28)
AL 2MG  0  4     B5    1( 17)
AL 2MG  0  4     B5    2( 20)
AL 2MG  0  4     B9    4(B20)
AL 2MG  0  4     B9    2(2-20)
AL 2MG  0  4     E2    5(160)
AL 2NA 20  4     A2    6( 83)
AL 2NA 20  4     A3    6( 83)
AL 20            A2    1( 59)
AL 20            A2    1( 62)
AL 20            A2    2( 83)
AL 20            A2    2(102)
AL 20            A5    4(C 2)
AL 20            C6    2(1-53)
AL 20            C6    4(A57)
AL 20            C6   11(144)
AL 20            G1   11(119)
AL 20 --0  2TI   E2    5(160)
AL 20  2         A2    1( 59)
AL 20  2         A2    1( 63)
AL 20  2         A2    2( 84)
AL 20  2         A2    2(102)
AL 20  2         A5    4(C 2)
AL 20  2         C6    2(1-54)
AL 20  2         C6    4(A58)
AL 20  3         A2    1( 59)
AL 20  3         A2    1( 63)
AL 20  3         A2    1( 64)
AL 20  3         A2    2( 84)
AL 20  3         A2    2( 85)
AL 20  3         A2    2(102)
AL 20  3         A2    4( 35)
AL 20  3         A5    4(C 2)
AL 20  3         A5    4(C 2)
AL 20  3         A9    3( 41)
AL 20  3         B1    2( 23)
AL 20  3         B2    1(  7)
AL 20  3         B2    2( 23)
AL 20  3         B3    1( 26)
AL 20  3         B3    1( 29)
AL 20  3         B5    1(  9)
AL 20  3         B5    2( 20)
AL 20  3         B9    2(2- 2)
AL 20  3         B9    4(B 2)
AL 20  3         D1    8( 61)
AL 20  3         D1   11( 99)
AL 20  3         D1   12( 81)
AL 20  3         D2    4( 33)
AL 20  3         D9    3( 41)
AL 20  3         D9    8( 67)
AL 20  3         E2    1( 88)
AL 20  3         E2    5(160)
AL 20  3         J2    1( 91)
AL 20  3         J2    1( 92)
AL 20  3----BE  0   F2    5(155)
AL 20  3----BF  0   F2    5(206)
AL 20  3----BE  0   M1   12(118)
AL203-BFO-MGO    F2    5(156)
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F  3LI 3         A2    1( 71)
F  3LI 3         A2    2( 98)
F  3LI 3         A2    2(105)
F  3LI 3         A5    4(C 2)
F  3N            B2    9( 28)
F  3N            B9    9( 32)
F  3N            C5   12(178)
F  3N    S       B5   12(180)
F  3O    P       C5   12(182)
F  3P            C5   12(182)
F  4LI 4         A2    1( 61)
F  4LI 4         A2    1( 72)
F  4LI 4         A2    2( 98)
F  4N  2         C5   12(178)
F  4N  2         C6    6(243)
F  4N  2         G1    2( 36)
F  4N  2         G1    6( 33)
F  4N  2         G2    6( 33)
F  4N  2         G9    2( 38)
F  4N  2         G9    2( 39)
F  4N  2         H1   10( 36)
F  4S            C5   12(173)
F  4XE           B5   12(167)
F  5I            B5   12(171)
F  5I            C5   12(171)
F  5P            C5   12(182)
F  6S            C5   12(173)
F  6SE           C5   12(174)
F  6TE           C5   12(175)
F  7I            C5   12(171)
FE               B2   12( 93)
FE  CL 2         B2   12( 95)
FE  O            B2   12( 96)
FE  O            B2   12( 96)
FE 20  3         B2   12( 97)
FF 30  4         B2   12( 97)
FF 20  4SI       B2   12( 96)
GO  H  2         A2    7( 93)
H                A2    1( 58)
H                A2    2(101)
H                A2    7( 91)
H                A5    4(C 1)
H                C5   12(165)
H                C6    2(1- 1)
H                C6    4(A 1)
H +              B5   12(165)
H +              C5   12(165)
H +              C6    7(107)
H -              C6   12(124)
H--              C5   12(165)
H   BE           C6   12(144)
H   D            C5   12(165)
H   F  2LI       B3   10( 40)
H   F  2LI       B9   10( 63)
H   I            B5   12(170)
H   I            C5   12(170)
H   I    O       B5   12(170)
H   I    O  3    B5   12(170)
H   K            A2    7( 92)
H   K    O       A2    7( 90)
H   K    O       C5   12(184)
H   LI           A2    1( 61)
H   LI           A2    8(870)
H   LI           A2    2( 97)
H   LI           A2    2(104)
H   LI           A2    7( 92)
H   LI           A5    4(C 2)
H   LI           A7    3( 41)
H   LI           B2    1( 19)
H   LI           B5    1( 22)
H   LI           B5    2( 20)
H   LI           C6   12(142)
H   LI   O       A2    1( 61)
H   LI   O       A2    1( 70)
H   LI   O       A2    2( 97)
H   LI   O       A2    2(105)
H   LI   O       A5    4(C 2)
H   LI   O       B2    1( 20)
H   LI   O       B2    2( 29)
H   LI   O       B3    1( 27)
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AL2O3--BEO--MGO           F2     5(207)      H  LI  O              B5    1( 22)
AL2O3-BEO-O2TI            F2     5(156)      H  LI  O              B5    2( 20)
AL2O3--BEO--O2TI          F2     5(207)      H  LI  O              B9    2(2-23)
AL2O3-BEO-O2ZR            F2     5(156)      H  LI  O              B9    4(B23)
AL2O3--BEO--O2ZR          F2     5(207)      H  LI  O              J2    1( 97)
AL 2O  3----MG  O         F2     5(156)      H  MG                 A2    1( 60)
AL 2O  3----MG  O         F2     5(208)      H  MG                 A2    2( 94)
AL2O3-MGO-O2TI            F2     5(156)      H  MG                 A2    2(104)
AL O3--MGO--O2TI          F2     5(209)      H  MG                 A5    4(C 2)
AL 2O  3----O  2TI        F2     5(156)      H  MG                 A7    2( 41)
AL2O3-O2TI-O2ZR           F2     5(157)      H  MG  O              A2    4( 36)
AL 2O  3----O  2TI        F2     5(209)      H  N                  A2    7( 91)
AL2O3--O2TI--O2ZR         F2     5(210)      H  N                  C5   12(175)
AL 2O  4ZR                F2     5(160)      H  N                  C6   12(146)
AL 2O  5SI                A2     6( 83)      H  N   O  2           B5   12(176)
AL 2O  5SI                A3     6( 83)      H  N   O  2           C5   12(176)
AL 2O  5SI                B2     7( 65)      H  N   O  2           C5   12(176)
AL 2O  5SI                B2     8( 99)      H  N   O  3           A2    7( 90)
AL 2O  5SI                B3     8( 99)      H  N   O  3           A2    7( 94)
AL 2O  5SI                B5     8(102)      H  N   O  3           B2    9( 29)
AL 2O  5SI                B9     8(166)      H  N   O  3           B3   10( 40)
AL 2O  5SI                B9     8(167)      H  N   O  3           B5   12(176)
AL 2O  5SI                B9     8(168)      H  N   O  3           B9    9( 32)
AL 2O  5TI                B2     7( 67)      H  N   O  3           B9   10( 81)
AL 2O  5TI                B2     8(101)      H  N  3               A2    7( 91)
AL 2O  5TI                B3     8(101)      H  N  3               B5   12(176)
AL 2O  5TI                B5     8(102)      H  N  3               C5   12(176)
AL 2O  5TI                B9     8(170)      H  N  3+              C5   12(176)
AL 2O  5ZR                A2     6( 83)      H  NA                 A2    7( 92)
AL 2O  5ZR                A3     6( 83)      H  NA                 B2    9( 18)
AL 4C  3                  A1    11(  1)      H  NA                 B9    9( 31)
AL 4C  3                  A1    11( 15)      H  NA  O              A2    7( 90)
AL 4C  3                  A1    11( 16)      H  NA  O              B2    9( 19)
AL 4C  3                  A1    12( 18)      H  O                  A2    7( 91)
AL 4C  3                  A1    12( 19)      H  O                  C5   12(165)
AL 4C  3                  A2     2(103)      H  O-                 A2    7( 90)
AL 4C  3                  A2     3(  3)      H  O -                B5   12(165)
AL 4C  3                  A2     3( 65)      H  O -                C5   12(165)
AL 4C  3                  A5     4(C 2)      H  O   NA             B9    9( 31)
AL 4C  3                  A8    11(  1)      H  O   NA             C5   12(184)
AL 4C  3                  A9    11( 15)      H  O  2               C5   12(165)
AL 4C  3                  B1     7( 13)      H  O  2+              C5   12(165)
AL 4C  3                  B1     8( 39)      H  O  2-              B5   12(165)
AL 4C  3                  B1    11( 21)      H  O  3P              B5   12(180)
AL 4C  3                  B1    11( 43)      H  O  3P --           B5   12(180)
AL 4C  3                  B2     3( 12)      H  O  3S -            B5   12(172)
AL 4C  3                  B2     8( 41)      H  O  3SE-            B5   12(174)
AL 4C  3                  B3     3( 12)      H  O  4P --           B5   12(180)
AL 4C  3                  B5     3( 16)      H  O  4S -            B5   12(172)
AL 4C  3                  B5     3( 21)      H  O  4SE-            B5   12(174)
AL 4C  3                  B9     3( 2[illegible]      H  O  7P  2---        B5   12(181)
AL 4C  3                  B9     3(2-37)     H  P                  C6   12(150)
AL 4C  3                  B9     4(B37)      H  S -                B5   12(172)
AL 4C  3                  B9     7(118)      H  SE-                B5   12(174)
AL 4C  3                  B9     8(135)      H  SR                 C6   12(156)
AL 4C  3                  B9    11( 40)      H  ZR                 B9   11(156)
AL 4C  3                  B9    11( 42)      H --ZR                B1   11( 94)
AL 4C  3                  B9    11( 43)      H --ZR                B9    5(243)
AL 4C  3                  D9     3( 33)      H --ZR                B9    5(244)
AL 4C  3                  D9     3( 34)      H --ZR                B9    5(245)
AL 43  3                  J2     4( 22)      H --ZR                B9    5(246)
AL 4C  3                  L1    11( 23)      H --ZR                B9    5(247)
AL 4C  3                  L1    11( 26)      H --ZR                B9   11(155)
AL 4C  3                  L8    11(  1)      H --ZR                B9   11(156)
AL 43A  O  7              B2    12( 89)      H --ZR                B9   11(156)
AL 4CL ?                  A2     2( 90)      H --ZR                B9   11(157)
AL 4O  3                  B9    11( 44)      H --ZR                F2    5(205)
AL 6BE  O 10              A2     4( 35)      H --ZR                F3   11( 95)
AL14CA12O 23              B2    12( 89)      H  2                  A2    1( 58)
AR                        C6     2(1-18)     H  2                  A2    2(101)
AR                        C6     4(A18)      H  2                  A2    7( 91)
AR+                       C6     6(239)      H  2                  A5    4(C 1)
AS  H  3                  A2     7( 91)      H  2                  A7    2( 41)
B                         A5     5( 39)      H  2                  B5   12(165)
B                         B9     5( 49)      H  2                  C5   12(165)
B                         B9     5( 50)      H  2                  C6    7(111)
B                         B9     5( 51)      H  2                  C6   11(157)
B                         C6     2(1- 5)     H  2                  C7   11( 83)
B                         C6     4(A 5)      H  2+                 C5   12(165)
B                         C6     5( 53)      H  2GO                A2    7( 93)
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B	+	C6	6(213)
B	BF 2	E2	5(150)
B	BR	A5	5(40)
B	BR	A5	5(40)
B	BR	A5	5(40)
B	BR	C6	2(1-42)
B	BR	C6	4(A45)
B	BR	C6	5(113)
B	BR	G9	5(43)
B	BR CL 2	A5	5(41)
B	BR CL 2	C6	5(121)
B	BR CL 2	G9	5(47)
B	BR F 2	A5	5(41)
B	BR F 2	C6	5(117)
B	BR F 2	G9	5(47)
B	BR 2	G9	5(47)
B	BR 2CL	A5	5(41)
B	BR 2CL	C6	5(123)
B	BR 2CL	G9	5(47)
B	BR 2F	A5	5(41)
B	BR 2F	C6	5(119)
B	BR 2F	G9	5(47)
B	BR3	C6	5(115)
B	CL	A	5(40)
B	CL	A5	5(40)
B	CL	C6	2(1-41)
B	CL	C6	4(A44)
B	CL	C6	5(95)
B	CL	G9	5(43)
B	CL F	A5	5(40)
B	CL F	C6	5(107)
B	CL F	G9	5(46)
B	CL F 2	A5	5(40)
B	CL F 2	C6	5(109)
B	CL O	A5	5(40)
B	CL O	C6	5(101)
B	CL O	G9	5(46)
B	CL 2	C6	5(97)
B	CL 2	G9	5(46)
B	CL 2F	A5	5(40)
B	CL 2F	C6	5(111)
B	CL 2F	G9	5(47)
B	CL 3	A5	5(40)
B	CL 3	C6	5(99)
B	CL 3	G9	5(46)
B	F	A5	5(40)
B	F	C6	2(1-40)
B	F	C6	4(A43)
B	F	C6	5(85)
B	F	G9	5(43)
B	F O	A5	5(40)
B	F O	C6	5(91)
B	F O	G9	5(46)
B	F 2	A5	5(40)
B	F 2	C6	5(87)
B	F 2	G9	5(46)
B	F 3	A5	5(40)
B	F 3	C6	5(89)
B	F 3	G9	5(46)
B	H	A5	5(39)
B	H	C6	2(1-39)
B	H	C6	4(A42)
B	H	C6	5(65)
B	H	G9	5(43)
B	H O 2	A5	5(39)
B	H O 2	C6	5(77)
B	H O 2	G9	5(45)
B	H 3	A2	7(91)
B	H 3	A5	5(39)
B	H 3	C6	5(67)
B	H 3	G9	5(45)
B	H 30 3	A2	7(90)
B	H 30 3	A5	5(39)
B	H 30 3	B9	5(79)
B	H 30 3	C6	5(81)
B	H 30 3	G9	5(46)
B	H 4K	A2	7(92)
B	H 4K	B2	11(92)
B	H 4K	B3	11(92)
B	H 4K	B9	11(177)

H	2LA	A2	7(93)
H	2MG	A2	2(94)
H	2MG	A2	2(104)
H	2MG	A2	7(92)
H	2MG	A5	4(C 2)
H	2MG	B2	1([illegible])
H	2MG	B2	[illegible]
H	2MG	B5	[illegible]
H	2MG	B5	[illegible]
H	2MG	B9	[illegible]
H	2MG	B9	4([illegible])
H	2MG	J2	1([illegible])
H	2MG O 2	A2	2(94)
H	2MG O 2	A2	2(104)
H	2MG O 2	B2	[illegible](14)
H	2MG O 2	B2	[illegible]
H	2MG O 2	B3	1(26)
H	2MG O 2	B5	1(17)
H	2MG O 2	B5	2(20)
H	2MG O 2	B9	2(2-13)
H	2MG O 2	B9	4(B13)
H	2MG O 2	J2	1(96)
H	2N	A2	7(91)
H	2N	C5	12(175)
H	2N NA	B2	9(19)
H	2N NA	B3	10(40)
H	2N NA	B9	9(31)
H	2N NA	B9	10(68)
H	20	A2	7(90)
H	20	B5	12(165)
H	20	C5	12(165)
H	20 2	A2	7(94)
H	20 2	B5	12(165)
H	20 2	C5	12(165)
H	20 2+	C5	12(166)
H	20 2MG	A5	4(C 2)
H	20 3S	B5	12(172)
H	20 3S	B5	12(172)
H	20 3SE	B5	12(174)
H	20 3TE	B5	12(175)
H	20 4P -	B5	12(181)
H	20 4S	B5	12(172)
H	20 4SE	B5	12(174)
H	20 7P 2--	B5	12(181)
H	20 7S 2	B5	12(173)
H	20 8S 2	B5	12(173)
H	20 +	C5	12(165)
H	2PR	A2	7(93)
H	2S	B5	12(172)
H	2S	C5	12(172)
H	2SE	B5	12(174)
H	2SF	C5	12(174)
H	2TE	C5	12(175)
H	2ZR	A2	7(93)
H	31 3N 2	B5	12(179)
H	3LI O 2	A2	2(97)
H	3LI O 2	B2	1(20)
H	3LI O 2	B2	2(29)
H	3LI O 2	B5	1(22)
H	3LI O 2	B5	2(20)
H	3LI O 2	B9	2(2-24)
H	3LI O 2	B9	4(B24)
H	3LI O 2	J2	1(97)
H	3LI O 3	J2	1(97)
H	3N	A2	7(91)
H	3N	B5	12(176)
H	3N	C5	12(175)
H	3N O	B5	12(177)
H	3N O 3S	B5	12(179)
H	3N O 4	B2	9(29)
H	3N O 4	B3	10(40)
H	3N O 4	B9	9(32)
H	3N O 4	B9	10(82)
H	30 2P	B5	12(181)
H	30 3P	B5	12(181)
H	30 3TE+	B5	12(175)
H	30 4P	B5	12(181)
H	30 7P 2-	B5	12(182)
H	3P	A2	7(91)
H	3P	B5	12(180)

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B   H   4LI                  A2        7( 92)
B   H   4LI                  B2       11( 89)
B   H   4LI                  B3       11( 89)
B   H   4LI                  B9       11(164)
B   H   4NA                  A2        7( 92)
B   H   4NA                  B2        9( 21)
B   H   4NA                  B2       11( 90)
B   H   4NA                  B3       11( 90)
B   H   4NA                  B9        9( 31)
B   H   4NA                  B9       11(169)
B   I   3                    A5        5( 41)
B   I   3                    C6        5(125)
B   I   3                    G9        5( 47)
B   N                        A2        7( 90)
B   N                        A5        5( 41)
B   N                        A5        5(150)
B   N                        B2        3( 13)
B   N                        B3        3( 13)
B   N                        B5        3( 16)
B   N                        B9        5(129)
B   N                        C6        2(1-44)
B   N                        C6        4(A47)
B   N                        C6        5(131)
B   N                        E2        5(150)
B   N                        G9        5( 43)
B   NA   O   2               B3       10( 40)
B   NA   O   2               B9        9( 31)
B   NA   O   2               B9       10( 73)
B   O                        A5        5( 39)
B   O                        C6        2(1-38)
B   O                        C6        4(A41)
B   O                        C6        5( 57)
B   O                        G9        5( 43)
B   O   2NA                  B2        9( 22)
B   S                        A5        5( 41)
B   S                        C6        2(1-43)
B   S                        C6        4(A46)
B   S                        C6        5(127)
B   S                        G9        5( 43)
B   TI                       A5        5(150)
B   TI                       E2        5(150)
B   TI  2                    A5        5(150)
B   ZR                       A5        5(150)
B   ZR                       F2        5(150)
B --ZR                       F2        5(195)
B  2                         A5        5( 39)
B  2                         C6        2(1-37)
B  2                         C6        4(A40)
B  2                         C6        5( 55)
B  2                         G9        5( 43)
B  2CL  4                    A5        5( 40)
B  2CL  4                    C6        5(101)
B  2CL  4                    G9        5( 46)
B  2H   6                    A2        7( 91)
B  2H   6                    A5        5( 39)
B  2H   6                    C6        5( 69)
B  2H   6                    G9        5( 45)
B  2MG                       B2        9( 16)
B  2MG                       B3       10( 40)
B  2MG                       B9        9( 31)
B  2MG                       B9       10( 64)
B  2O   2                    A5        5( 39)
B  2O   2                    C6        5( 59)
B  2O   2                    G9        5( 45)
B  2O   3                    A2        7( 90)
B  2O   3                    A5        5( 39)
B  2O   3                    B9        5( 62)
B  2O   3                    C6        5( 61)
B  2O   3                    C6        5( 63)
B  2O   3                    G9        5( 45)
B  2O   3----CA   O          A2        6( 79)
B  2O   3----K   2O          A2        6( 78)
B  2O   3----LI  2O          A2        6( 77)
B  2O   3----LI  2O          F2        5(15 )
B  2O   3----LI  2O          F2        5(213)
B  2O   3----MG   O          F2        5(157)
B  2O   3----MG   O          F2        5(214)
B  2O   3NA  2O              A2        6( 77)
B  2O   3----O    PB         A2        6( 80)
B  2TI                       A5        5(150)

H   3P                       C5       12(180)
H   3P  +                    C5       12(180)
H   3U                       A2        7( 93)
H   4CL   O   8P             B5       12(182)
H   4CL   P                  B5       12(182)
H   4I    N                  B5       12(179)
H   4I    P                  B5       12(182)
H   4N    O  +               B5       12(177)
H   4N    TE                 B5       12(180)
H   4N   2                   A2        7( 91)
H   4N   2                   B5       12(176)
H   4N   2                   C5       12(176)
H   4N   2O   2              B5       12(177)
H   4N   2O   3              A2        7( 94)
H   4N   2O   3              B2        9( 27)
H   4N   2O   3              B5       12(177)
H   4N   2O   3              B9        9( 32)
H   4N   2O   4              B5       12(177)
H   4N   4                   B5       12(176)
H   4N  +                    B5       12(176)
H   4O   6TE--               B5       12(175)
H   4O   7P   2              B5       12(182)
H   4P   2                   A2        7( 91)
H   4P   2                   B5       12(180)
H   4P   2                   C5       12(180)
H   4SI                      A2        7( 91)
H   5N    O                  B2        9( 27)
H   5N    O                  B3       10( 40)
H   5N    O                  B5       12(177)
H   5N    O                  B9        9( 32)
H   5N    O                  B9       10( 78)
H   5N    O   3S             B5       12(179)
H   5N    O   4S             B5       12(179)
H   5N    O   5S             B5       12(179)
H   5N    S                  B5       12(179)
H   5N    SE                 B5       12(180)
H   5N   2+                  B5       12(176)
H   5N   3O   2              B5       12(178)
H   5O   6TE                 B5       12(175)
H   6N    O   4P             B5       12(183)
H   6N   2O                  B5       12(177)
H   6N   2O                  C5       12(177)
H   6O   6TE                 B5       12(175)
H   6SI  2                   A2        7( 91)
H   7N    O   6              B2        9( 27)
H   7N    O   6              B3       10( 40)
H   7N    O   6              B9        9( 32)
H   7N    O   6              B9       10( 83)
H   8N   2O                  B2        9( 26)
H   8N   2O                  B3       10( 40)
H   8N   2O                  B9        9( 32)
H   8N   2O                  B9       10( 77)
H   8N   2O   3S             B5       12(179)
H   8N   2O   4S             B5       12(179)
H   8N   2O   6S             B5       12(179)
H   8N   2O   8S   2         B5       12(179)
H   9N   2O   4P             B5       12(183)
H  10N   2O   4S             B5       12(179)
H  10N   4O   4S             B5       12(180)
H  12N   3O   4P             B5       12(183)
H  12N   4O   5S             B5       12(180)
H  18N   3O   5P             B5       12(183)
HE                           C6        2(1- 2)
HE                           C6        4(A 2)
HE+                          C6        6(207)
HG                           B1        9( 29)
HG                           B2        9( 29)
HG                           B9        9( 32)
HG+                          C6        6(261)
HG   O                       B2        9( 30)
HG   O                       B9        9( 32)
HG   O                       B9       10( 84)
I                            C5       12(169)
I  +                         C5       12(169)
I  +                         C6        6(255)
I  -                         B5       12(170)
I  -                         C5       12(170)
I     K                      B2        7( 71)
I     K                      G9       10( 19)
I     K    O   3             B2        9( 26)
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B   2TI                           E2       5(150)
B   2ZR                           A5       5(150)
B   2ZR                           E2       5(150)
B   3CL  30   3                   A5       5( 40)
B   3CL  30   3                   C6       5(105)
B   3CL  30   3                   G9       5( 46)
B   3F   30   3                   A5       5( 40)
B   3F   30   3                   C6       5( 93)
B   3F   30   3                   G9       5( 46)
B   3H   2N   3                   C6       5(133)
B   3H   30   6                   A5       5( 40)
B   3H   30   6                   C6       5( 83)
B   3H   30   6                   G9       5( 46)
B   3H   6N   3                   A5       5( 41)
B   3H   6N   3                   G9       5( 47)
B   4C                            A5       5( 41)
B   4C                            A5       5(150)
B   4C                            B1       3( 11)
B   4C                            B2       3( 11)
B   4C                            B5       3( 16)
B   4C                            B9       5(135)
B   4C                            E2       5(150)
B   4H 10                         A2       7( 91)
B   4MG                           B2       9( 16)
B   4MG                           B3      10( 40)
B   4MG                           B9       9( 31)
B   4MG                           B9      10( 65)
B   4NA  20   7                   B2       9( 22)
B   4NA  20   7                   B3      10( 40)
B   4NA  20   7                   B9       9( 31)
B   4NA  20   7                   B9      10( 73)
B   5H   8K     0  12             B9       6(266)
B   5H   9                        A2       7( 91)
B   5H   9                        A5       5( 39)
B   5H   9                        B9       5( 71)
B   5H   9                        C6       5( 72)
B   5H   9                        G9       5( 45)
B   5H 10NA     0  13             B9       6(264)
B   5H 11                         A2       7( 91)
B   5H 12N      0  12             B9       6(268)
B   5TI  2                        A5       5(150)
B   5TI  2                        E2       5(150)
B   6BE                           E2       5(150)
B   6H 10                         A2       7( 91)
B  10H 14                         A2       7( 91)
B  10H 14                         A5       5( 39)
B  10H 14                         B9       5( 74)
B  10H 14                         C6       5( 75)
B  10H 14                         G9       5( 45)
B  12ZR                           A5       5(150)
B  12Z-                           F2       5(150)
B  13C   2                        E2       5(150)
BA                                B2      12( 87)
BA   CL  2                        B2      12( 87)
BA   F   2                        B2      12( 87)
BA   H                            C6      12(158)
BA   0                            B2      12( 87)
BE                                A2       1( 58)
BE                                A2       2(101)
BE                                A5       4(C 1)
BE                                B1       1( 11)
BE                                B1       2( 24)
BE                                B2       2( 24)
BE                                B3       1( 26)
BE                                B3       1( 29)
BE                                B5       1( 12)
BE                                B5       2( 20)
BE                                B9       2(2- 7)
BE                                B9       4(B 7)
BE                                C6       2(1- 4)
BE                                C6       4(A 4)
BE                                D2       1( 48)
BE                                D2       1( 54)
BE+                               C6       6(211)
BE   AL  20   4                   B5       1( 12)
BE   C   2                        A2       2( 93)
BE   C   2                        A2       2(103)
BE   C   2                        A5       4(C 2)
BE   C   2                        A7       3(  4)
BE   CL                           A2       1( 60)
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I    K    0   3                   B3      10( 40)
I    K    0   3                   B9      10( 76)
I    LI                           B7       6( 54)
I    LI                           G9      10( 19)
I    NA                           G9      10( 19)
I    0  -                         B5      12(170)
I    0  3-                        B5      12(170)
I    0   4+                       B5      12(170)
I    RB                           G9      10( 19)
I   2                             B5      12(170)
I   2                             C5      12(170)
I   2MG                           B7       6( 54)
I   20   5                        A2       7( 94)
I   20   5                        C5      12(170)
I   3-                            B5      12(170)
I   3P                            B5      12(182)
I   3P                            C5      12(182)
K                                 B2       7( 69)
K  +                              C5      12(184)
K  +                              C6       6(257)
K    H                            C6      12(152)
K    N     0   3                  A9       7( 10)
K    N     0   3                  B1       7(  3)
K    N     0   3                  B2       9( 25)
K    N     0   3                  B9       9( 32)
K    NA  2                        B2       9( 17)
K    NA  2                        B9       9( 31)
K    0   2                        A2       7( 95)
K    0   2                        B2       7( 69)
K    0   3                        A2       7( 95)
K   20                            A2       7( 95)
K   20   2                        A2       7( 95)
K   20   3                        A2       7( 95)
K   20   5SI  2                   B2       7( 66)
K   20   9SI  4                   B2       7( 66)
LI                                A2       1( 58)
LI                                A2       2(101)
LI                                A5       4(C 1)
LI                                B1       1( 19)
LI                                B1       5(175).
LI                                B2       1( 19)
LI                                B2       2( 28)
LI                                B2       2( 28)
LI                                B2       3( 63)
LI                                B2       5(175)
LI                                B3       1( 27)
LI                                B5       1( 22)
LI                                B5       1( 32)
LI                                B5       2( 20)
LI                                B9       2(2-21)
LI                                B9       4(B21)
LI                                B9       5(227)
LI                                C6       2(1- 3)
LI                                C6       4(A 3)
LI                                D2       1( 48)
LI+                               C6       6(209)
LI--MG                            F2       5(198)
LI   N                            A2       1( 61)
LI   0                            A2       1( 61)
LI   0                            A2       1( 70)
LI   0                            A2       2( 97)
LI   0                            A2       2(104)
LI   0                            A5       4(C 2)
LI   0                            C6      12(160)
LI   C                            G1      11(118)
LI--0                             D2       2( 64)
LI   0   3                        A2       7( 95)
LI  2                             A2       1( 61)
LI  2                             A2       1( 70)
LI  2                             A2       2( 96)
LI  2                             A2       2(104)
LI  2                             A5       4(C 2)
LI  2                             A7       2( 41)
LI  2                             B5       1( 22)
LI  2                             C6       1(105)
LI  2                             C6       2(1-19)
LI  2                             C6       4(A19)
LI  2                             G2       1( 42)
LI  2                             G9       2( 50)
LI  20                            A2       1( 61)
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BE   CL                A2      1( 68)
BE   CL                A2      2( 92)
BE   CL                A2      2(103)
BE   CL                A5      4(C 2)
BE   CL                C6      1(112)
BE   CL                C6      2(1-24)
BE   CL                C6      4(A24)
BE   CL                G2      1( 42)
BE   CL                G9      2( 50)
BE   CL   F            C6      2(1-49)
BE   CL   F            C6      4(A53)
BE   CL   F            G2      1( 43)
BE   CL   F            G9      2( 51)
BE   CL 2              A1      4( 28)
BE   CL 2              A2      1( 60)
BE   CL 2              A2      1( 68)
BE   CL 2              A2      2( 92)
BE   CL 2              A2      2( 93)
BE   CL 2              A2      2(103)
BE   CL 2              A2      4( 35)
BE   CL 2              A2      4( 37)
BE   CL 2              A2      4( 37)
BE   CL 2              A2      7( 90)
BE   CL 2              A3      4( 37)
BE   CL 2              A3      4( 37)
BE   CL 2              A5      4(C 2)
BE   CL 2              B5      1( 12)
BE   CL 2              C6      2(1-48)
BE   CL 2              C6      4(A52)
BE   CL 2              G2      1( 43)
BE   CL 2              G9      2( 51)
BE   F   2             A2     12( 22)
BE   F                 A2      1( 60)
BE   F                 A2      1( 68)
BE   F                 A2      2( 92)
BE   F                 A2      2(103)
BE   F                 A5      4(C 2)
BE   F                 C6      1(111)
BE   F                 C6      2(1-23)
BE   F                 C6      4(A23)
BE   F                 D3      8(114)
BE   F                 G2      1( 42)
BE   F                 G2      4( 45)
BE   F                 G3      8(109)
BE   F                 G9      2( 50)
BE   F                 G9      4( 47)
BE--F --0              D1      8( 55)
BE--F --0              M1      8( 55)
BE--F --0              M1     10( 55)
BE--F --0              M8      8( 56)
BE   F   2             A2      1( 60)
BE   F   2             A2      1( 68)
BE   F   2             A2      2( 92)
BE   F   2             A2      2(103)
BE   F   2             A2      3( 65)
BE   F   2             A2      4( 35)
BE   F   2             A2     10( 43)
BE   F   2             A3     10( 43)
BE   F   2             A3     12(120)
BE   F   2             A5      4(C 2)
BE   F   2             B3     11(113)
BE   F   2             B5      1( 12)
BE   F   2             B7      7( 96)
BE   F   2             B9      7(117)
BE   F   2             B9     11(158)
BE   F   2             C6      2(1-47)
BE   F   2             C6      4(A51)
BE   F   2             C6     12(138)
BE   F   2             D2      4( 35)
BE   F   2             D3     11(113)
BE   F   2             G2      1( 43)
BE   F   2             G7     12( 85)
BE   F   2             G9      2( 51)
BE   F   2             J8     11( 84)
BE   F   2             J8     12( 73)
BE   F   2             M1      8( 55)
BE   F   2             M1     10( 55)
BE   F   2             M9     10( 57)
BE   F   2----BE   0   A1     11(109)
BE   F   2----BE   0   A1     11(110)
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LI 20                  A2      2( 97)
LI 20                  A2      2(104)
LI 20                  A2      3( 65)
LI 20                  A2      7( 95)
LI 20                  A5      4(C 2)
LI 20                  B2      1( 19)
LI 20                  B2      2( 28)
LI 20                  B3      1( 27)
LI 20                  B5      2( 20)
LI 20                  B9      2(2-22)
LI 20                  B9      4(B22)
LI 20                  C6     11(148)
LI 20                  E2      5(160)
LI 20                  G1     11(118)
LI 20                  J2      1( 97)
LI 20  2               A2      2( 97)
LI 20  2               A2      2(104)
LI 20  2               A2      7( 95)
LI 20  2               A5      4(C 2)
LI 20  2               C6     11(150)
LI 20  2               G1     11(118)
LI 20  3SI             A2      6( 83)
LI 20  3SI             A3      [illegible]( 83)
LI 20  3TI             B2      7( 66)
LI 20  3TI             B2      8( 93)
LI 20  3TI             B3      8( 93)
LI 20  3TI             B5      8(102)
LI 20  3TI             B9      8(144)
LI 20  5SI 2           B2      7( 64)
LI 20  7SI 3           B2      7( 64)
LI 3N                  A2      1( 61)
LI 3N                  A2      2(100)
LI 3N                  A2      2(105)
LI 3N                  A2      3(  5)
LI 3N                  A3      3(  5)
LI 3N                  A5      4(C 2)
LI 3N                  B2      3( 13)
LI 3N                  B5      3( 16)
LI 3N                  B5      3( 21)
LI 3N                  B9      3( 22)
LI 3N                  B9      3(2-28)
LI 3N                  B9      4(B28)
LI 3N                  D9      3( 47)
LI 3N                  J2      4( 24)
MG                     A2      1( 58)
MG                     A2      2(101)
MG                     A5      4(C 1)
MG                     B2      1( 14)
MG                     B2      2( 25)
MG                     B3      1( 26)
MG                     B5      1( 17)
MG                     B5      2( 20)
MG                     B9      2(2- 9)
MG                     B9      4(B 9)
MG                     C6      2(1-12)
MG                     C6      4(A12)
MG                     D2      1( 48)
MG+                    C6      6(227)
MG   C   2             A2      3(  5)
MG   0                 A2      1( 60)
MG   0                 A2      1( 69)
MG   0                 A2      2( 94)
MG   0                 A2      2(103)
MG   0                 A2      4( 36)
MG   0                 A5      4(C 2)
MG   0                 B1      2( 25)
MG   0                 B2      1( 14)
MG   0                 B2      2( 25)
MG   0                 B3      1( 26)
MG   0                 B5      1( 17)
MG   0                 B5      2( 20)
MG   0                 B9      2(2-10)
MG   0                 B9      2(2-11)
MG   0                 B9      4(B10)
MG   0                 B9      4(B11)
MG   0                 C6      1(121)
MG   0                 C6      2(1-25)
MG   0                 C6      4(A25)
MG   0                 D1     12( 83)
MG   0                 E2      5(160)
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BE F 2----BE O	M1	10(56)
BE F 2----BE O	M1	11(103)
BE F 2----BE O	M9	11(109)
BE F 2----BE O	M9	11(110)
BE F 2----F LI	F2	5(163)
BE F 2----F LI	F2	5(218)
BE F 2----F 2MG	F2	5(166)
BE F 2----F 2MG	F2	5(224)
BE F 2----F 2MG	F2	5(225)
BE F 4LI 2	B1	11(75)
BE F 4LI 2	B9	11(78)
BE F 4LI 2	B9	11(163)
BE H	A2	1(60)
BE H	A2	2(91)
BE H	A2	2(103)
BE H	A5	4(C 2)
BE H	A7	2(41)
BE H 2	A2	7(92)
BE H 2	B5	1(12)
BE H 2	J2	1(100)
BE H 2	J8	3(55)
BE H 2O 2	[illegible]	1([illegible])
BE H 2O 2	A2	1(67)
BE H 2O 2	A2	2(91)
BE H 2O 2	A2	2(92)
BE H 2O 2	A2	2(103)
BE H 2O 2	A5	4(C 2)
BE H 2O 2	B5	1(12)
BE H 2O 2	J2	1(94)
BE O	A2	1(60)
BE O	A2	1(67)
BE O	A2	2(91)
BE O	A2	2(103)
BE O	A2	4(35)
BE O	A3	12(120)
BE O	A5	4(C 2)
BE O	B1	2(24)
BE O	B2	2(24)
BE O	B3	1(26)
BE O	B5	1(12)
BE O	B5	2(20)
BE O	B9	2(2- 8)
BE O	B9	4(B 8)
BE O	C6	1(115)
BE O	C6	2(1-22)
BE O	C6	4(A2[illegible]
BE O	D2	1(5[illegible]
BE O	D2	1(54)
BE O	D2	4(31)
BE O	E2	5(160)
BE O	G2	1(42)
BE O	G9	2(50)
BE O	J2	1(94)
BE O	M1	8(55)
BE--O	D2	2(63)
BE--O	D3	2(63)
BEO-MGO-O2ZR	F2	5(157)
BEO--MGO--O2ZR	F2	5(211)
BE O --O 2TI	F2	5(157)
BE O --O 2TI	F2	5(211)
BEO-O2TI-O2ZR	F2	5(157)
BEO--O2TI--O2ZR	F2	5(212)
BE--SI	F2	5(196)
BE--ZR	F2	5(197)
BE 2	A2	1(60)
BE 2	A2	1(67)
BE 2	A2	2(91)
BE 2	A2	2(103)
BE 2	A5	4(C 2)
BE 2	A7	2(41)
BE 2C	A2	2(93)
BE 2C	A2	2(103)
BE 2C	A5	4(C 2)
BE 2C	B2	3(11)
BE 2C	B5	3(16)
BE 2C	B5	3(21)
BE 2C	B9	3(22)
BE 2C	B9	3(2-34)
BE 2C	B9	4(B34)
BE 2C	D9	3(42)

MG O	G2	1(42)
MG O	G9	2(50)
MG O	J2	1(96)
MG--O	D2	2(64)
MG O --F 2MG	F2	5(158)
MG O --O 2TI	F2	5(158)
MG O --O 2TI	F2	5(214)
MGO-O2TI-O2ZR	F2	5(158)
MGO--O2TI--O2ZR	F2	5(216)
MG O --O 2ZR	F2	5(158)
MG O --O 2ZR	F2	5(215)
MG--SI	F2	5(199)
MG--TI	F2	5(200)
MG--ZR	F2	5(201)
MG O 2	A2	1(60)
MG O 2	A2	1(69)
MG O 2	A2	2(94)
MG O 2	A2	2(104)
MG O 2	A5	4(C 2)
MG O 3SI	A2	6(83)
MG O 3SI	A3	6(83)
MG O 3SI	B2	7(65)
MG O 3SI	B2	[illegible](94)
MG O 3SI	B3	8(94)
MG O 3SI	B5	8(102)
MG O 3SI	B9	8(146)
MG O 3TI	A2	6(83)
MG O 3TI	A3	6(83)
MG O 3TI	B2	7(67)
MG O 3TI	B2	8(95)
MG O 3TI	B3	8(95)
MG O 3TI	B5	8(102)
MG O 3TI	E2	5(160)
MG O 4TI	B9	8(150)
MG O 4W	B2	7(68)
MG O 4W	B2	8(93)
MG O 4W	B3	8(93)
MG O 4W	B5	8(102)
MG O 4W	B9	8(143)
MG O 5TI	B2	8(95)
MG O 5TI	B3	8(95)
MG O 5TI 2	A2	6(83)
MG O 5TI 2	A3	6(83)
MG O 5TI 2	B2	7(67)
MG O 5TI 2	B5	8(102)
MG O 5TI 2	B9	8(152)
MG 2	A2	1(60)
MG 2	A2	1(69)
MG 2	A2	2(93)
MG 2	A2	2(103)
MG 2	A5	4(C 2)
MG 2	A7	2(41)
MG 2C 3	A2	3(5)
MG 2O 4SI	A2	6(83)
MG 2O 4SI	A3	6(83)
MG 2O 4SI	B2	7(64)
MG 2O 4SI	B2	8(94)
MG 2O 4SI	B3	8(94)
MG 2O 4SI	B5	8(102)
MG 2O 4SI	B9	8(148)
MG 2O 4TI	A2	6(83)
MG 2O 4TI	A[illegible]	6(83)
MG 2O 4TI	B2	7(66)
MG 2O 4TI	B2	8(96)
MG 2O 4TI	B3	8(96)
MG 2O 4TI	B5	8(102)
MG 2O 4TI	B9	8(154)
MG 3N 2	A2	2(96)
MG 3N 2	A2	2(104)
MG 3N 2	A2	3(4)
MG 3N 2	A3	3(4)
MG 3N 2	A5	4(C 2)
MG 3N 2	B2	3(14)
MG 3N 2	B3	3(14)
MG 3N 2	B5	3(16)
MG 3N 2	B5	3(21)
MG 3N 2	B9	3(22)
MG 3N 2	B9	3(2-30)
MG 3N 2	B9	4(B30)
MG 3N 2	D9	3(45)

BE 2C	J2	4(20)
BE 2CL 4	A2	1(60)
BE 2CL 4	A2	1(69)
BE 2CL 4	A2	2(93)
BE 2CL 4	A2	2(103)
BE 2CL 4	A2	4(37)
BE 2CL 4	A3	4(37)
BE 2CL 4	A5	4(C 2)
BE 2F 20	A3	12(120)
BE 2F 20	A9	12(121)
BE 2F 20	C6	11(146)
BE 2F 20	G7	11(119)
BE 20 2	D2	1(54)
BE 20 4SI	A2	6(83)
BE 20 4SI	A3	6(83)
BE 20 4SI	B2	7(64)
BE 20 4SI	B2	8(101)
BE 20 4SI	B3	8(101)
BE 20 4SI	B5	8(102)
BE 20 4SI	B9	8(169)
BE 3N 2	A2	2(93)
BE 3N 2	A2	2(103)
BE 3N 2	A2	3(4)
BE 3N 2	A3	3(4)
BE 3N 2	A5	4(C 2)
BE 3N 2	B1	8(44)
BE 3N 2	B2	3(13)
BE 3N 2	B2	8(50)
BE 3N 2	B5	3(16)
BE 3N 2	B5	3(21)
BE 3N 2	B9	3(22)
BE 3N 2	B9	3(2-29)
BE 3N 2	B9	4(B29)
BE 3N 2	B9	8(48)
BE 3N 2	B9	8(134)
BE 3N 2	D9	3(43)
BE 3N 2	J2	4(25)
BE 30 3	D2	1(54)
BE 40 4	D2	1(54)
BE 50 5	D2	1(54)
BE 60 6	D2	1(54)
BR	C5	12(168)
BR+	C5	12(168)
BR+	C6	6(247)
BR-	B5	12(168)
BR-	C5	12(168)
BR CL	A2	7(94)
BR CL	B5	12(169)
BR CL	C5	12(169)
BR CS	G9	10(19)
BR F 3	B5	12(169)
BR F 5	B5	12(169)
BR F 5	C5	12(169)
BR H	B5	12(169)
BR H	C5	12(169)
BR H O	B5	12(169)
BR H O 3	B5	12(169)
BR H 4N	B5	12(179)
BR H 4P	B5	12(182)
BR H 5N 2	B5	12(179)
BR I	B5	12(171)
BR I	C5	12(171)
BR K	B2	7(71)
BR K	B2	11(91)
BR K	B3	11(91)
BR K	G9	10(19)
BR K O 3	B2	9(26)
BR K O 3	B3	10(40)
BR K O 3	B9	9(32)
BR K O 3	B9	10(75)
BR LI	B7	6(54)
BR LI	G9	10(19)
BR N O	C5	12(179)
BR NA	G9	10(19)
BR O -	B5	12(169)
BR O 2	C5	12(169)
BR O 3-	B5	12(169)
BR RB	G9	10(19)
BR 2	B5	12(168)
BR 2	B9	11(175)
MG 3N 2	J2	4(25)
MO+	C6	6(253)
N	A2	2(101)
N	A2	7(90)
N	A5	4(C 1)
N	C5	12(175)
N	C6	2(1- 7)
N	C6	4(A 7)
N +	C5	12(175)
N +	C6	6(217)
N NA O 3	B2	9(23)
N NA O 3	B9	9(31)
N NA 3	B5	3(16)
N NA 3	B7	3([illegible])
N O	A2	7(94)
N O	C5	12(175)
N O +	C5	12(175)
N O +	C6	12(136)
N O 2	A2	7(94)
N O 2+	C5	12(175)
N O 2-	B5	12(175)
N O 3-	B5	12(175)
N P	C5	12(183)
N TI	A2	3(6)
N TI	A3	3(6)
N TI	A5	4(C 2)
N TI	B2	3(14)
N TI	B3	3(14)
N TI	B5	3(16)
N TI	B5	3(21)
N TI	B9	3(22)
N TI	B9	3(2-32)
N TI	B9	4(B32)
N TI	D9	3(50)
N ZR	B2	5(179)
N ZR	B9	5(250)
N 2	A2	2(101)
N 2	A5	4(C 1)
N 2	C5	12(175)
N 2	C6	3(1-66)
N 2	C6	4(A48)
N 20	C5	12(175)
N 20 3	A2	7(94)
N 20 3	B5	12(175)
N 20 4	A2	7(94)
N 20 4	B5	12(175)
N 20 4	C5	12(175)
N 20 5	A2	7(94)
N 20 5	B5	12(175)
N 2P	C6	12(132)
N 3+	C5	12(175)
N 3-	B5	12(175)
N 3-	C5	12(175)
N 4SI 3	B2	3(14)
N 4SI 3	B2	12(101)
N 4SI 3	B3	3(14)
N 4SI 3	B5	3(16)
N 5P 3	B5	12(183)
NA	B2	9(16)
NA	B9	9(31)
NA	C6	2(1-11)
NA	C6	4(A11)
NA H	C6	12(148)
NA O 2	A2	7(95)
NA O 2	B2	9(18)
NA O 2	B3	10(40)
NA O 2	B9	9(31)
NA O 2	B9	10(67)
NA O 3	A2	7(95)
NA 20	A2	7(95)
NA 20	B1	9(18)
NA 20	B2	9(18)
NA 20	B9	9(31)
NA 20 I	B2	9(18)
NA 20 2	A2	7(95)
NA 20 2	B3	10(40)
NA 20 2	B9	9(31)
NA 20 2	B9	10(66)
NA 20 3SI	A2	6(83)
NA 20 3SI	A3	6(83)

BR 2	C5	12(168)
BR 2+	C5	12(168)
BR 2MG	B7	6(54)
BR 2PB	B2	6(53)
BR 2PB	B3	6(53)
BR 3-	B5	12(168)
BR 30 P	B5	12(182)
B- 30 P	C5	12(182)
BR 3P	B5	12(182)
BR 3P S	B5	12(182)
BR 3P S	C5	12(182)
BR 4TE	B5	12(175)
BR 5-	B5	12(168)
C	A2	2(101)
C	A5	4(C 1)
C	B5	12(183)
C	B9	3(2-39)
C	B9	4(B39)
C	C5	12(183)
C	C6	2(1- 6)
C	C6	4(A 6)
C +	C6	6(215)
C --FE	B2	12(95)
C FE3	B2	12(95)
C H O 3-	B5	12(183)
C H 2N 2	A2	7(91)
C H 2O 3	B5	12(183)
C H 5N	A2	7(91)
C H 6N 2	A2	7(91)
C O	C5	12(183)
C O 2	A2	7(90)
C O 2	B5	12(183)
C O 2	C5	12(183)
C O 3--	B5	12(183)
C SI	B2	3(12)
C SI	B2	12(99)
C SI	B3	3(12)
C SI	B5	3(16)
C TI	A2	3(6)
C TI	A2	3(6)
C TI	A5	4(C 2)
C TI	B2	3(13)
C TI	B5	3(16)
C TI	B5	3(21)
C TI	B9	3(22)
C TI	B9	3(2-38)
C TI	B9	4(B38)
C TI	D9	3(48)
C TI	D9	3(49)
C 2CA	B2	12(88)
C 2CR 3	B2	12(92)
C 2CR 5	B2	12(92)
C 2H 5N	A2	7(91)
C 2H 8N 2	A2	7(91)
C 2H 8N 2	A2	7(91)
C 2LI 2	A2	2(100)
C 2LI 2	A2	2(105)
C 2LI 2	A3	3(5)
C 2LI 2	A5	4(C 2)
C 2LI 2	B2	3(11)
C 2LI 2	B5	3(16)
C 2LI 2	B5	3(21)
C 2LI 2	B9	3(22)
C 2LI 2	B9	4(B33)
C 2LI 2	D9	3(46)
C 2LI 2	J2	4(18)
C 2MG	A2	2(96)
C 2MG	A2	2(104)
C 2MG	A5	4(C 2)
C 2MG	B2	3(12)
C 2MG	B3	3(12)
C 2MG	B5	3(16)
C 2MG	B5	3(21)
C 2MG	B9	3(22)
C 2MG	B9	3(2-35)
C 2MG	B9	4(B35)
C 2MG	J2	4(21)
C 2NA 2	B2	3(12)
C 2NA 2	B3	3(12)
C 2NA 2	B5	3(16)

NA 20 3SI	B2	9(23)
NA 20 3SI	B9	9(31)
NA 20 3TI	B2	9(24)
NA 20 3TI	B9	9(31)
NA 20 5SI 2	B2	9(24)
NA 20 5SI 2	B9	9(31)
NA 20 5TI 2	B2	9(24)
NA 20 5TI 2	B9	9(31)
NA 20 5SI 2	A2	6(83)
NA 20 5SI 2	A3	6(83)
NA 20 7TI 3	B2	9(25)
NA 20 7TI 3	B9	9(31)
NA 20 7TI 3	B9	9(31)
NA 30 7SI 2	A2	6(83)
NA 30 7SI 2	A3	6(83)
NA 40 4SI	A2	6(83)
NA 40 4SI	A3	6(83)
NA 40 4SI	B2	9(24)
NA 40 4SI	B9	9(31)
NA+	C5	12(184)
NA+	C6	6(225)
NE	C6	2(1-10)
NE	C6	4(A10)
NE+	C6	6(223)
O	A2	1(58)
O	A2	2(101)
O	A2	7(94)
O	A5	4(C 1)
O	C5	12(165)
O	C6	2(1- 8)
O	C6	4 A 8)
O	D2	1, 54)
O +	C5	12(165)
O +	C6	6(219)
O -	C5	12(165)
O -	C6	12(126)
O PB	B2	6(52)
O PB	B2	8(97)
O PB	B2	8(98)
O PB	B3	8(97)
O PB	B3	8(98)
O PB	B5	8(102)
O PB	B5	8(102)
O PB	B9	8(158)
O PB	B9	8(160)
O S	C5	12(171)
O TI	B2	5(176)
O TI	B9	5(231)
O 2	A2	1(58)
O 2	A2	2(101)
O 2	A2	7(94)
O 2	A5	4(C 1)
O 2	A7	2(41)
O 2	B5	12(165)
O 2	C5	12(165)
O 2	C6	7(113)
O 2	D2	1(54)
O 2+	C5	12(165)
O 2+	C6	12(134)
O 2PB	B2	6(53)
O 2PB	B2	8(98)
O 2PB	B3	6(53)
O 2PB	B3	8(98)
O 2PB	B5	8(102)
O 2PB	B9	8(161)
O 2S	B5	12(171)
O 2S	C5	12(171)
O 2SE	B5	12(174)
O 2SI	B2	7(68)
O 2SI	B2	12(99)
O 2SI	B2	12(100)
O 2TE	B5	12(175)
O 2TI	A2	3(5)
O 2TI	A3	3(5)
O 2TI	A5	4(C 2)
O 2TI	B2	5(177)
O 2TI	B2	5(178)
O 2TI	B9	5(237)
O 2TI	B9	5(239)
O 2TI	E2	5(160)

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C   2TI 2           B9      3(2-33)
C   3CR 7           B2     12( 92)
C   3MG 2           A2      2( 96)
C   3MG 2           A2      2(104)
C   3MG 2           A5      4(C 2)
C   3MG 2           B2      3( 12)
C   3MG 2           B5      3( 16)
C   3MG 2           B5      3( 21)
C   3MG 2           B9      3( 22)
C   3MG 2           B9      3(2-36)
C   3MG 2           B9      4(B36)
C   3MG 2           J2      4( 21)
C   4H 12N   4      A2      7( 91)
C   6CR23           B2     12( 93)
CA                  B2     12( 87)
CA   CL 2           B2     12( 88)
CA   F  2           B2     12( 88)
CA   FE 20   4      B2     12( 89)
CA   H              C6     12(154)
CA   O              B2     12( 88)
CA   O  3SI         A2      6( 83)
CA   O  3SI         A3      6( 83)
CA   O  3SI         B2     12( 90)
CA   O  3TI         A2      6( 83)
CA   O  3TI         A3      6( 83)
CA 2FE  20   5      B2     12( 90)
CA 20   4SI         A2      6( 83)
CA 20   4SI         A3      6( 83)
CA 20   4SI         B2     12( 90)
CA 30   5SI         A2      6( 83)
CA 30   5SI         A3      6( 83)
CA 30   5SI         B2     12( 91)
CA 30   7SI 2       B2     12( 91)
CE  H   2           A2      7( 93)
CL                  A2      1( 58)
CL                  A2      2(101)
CL                  A2      7( 90)
CL                  A5      4(C 1)
CL                  C5     12(167)
CL                  C6      2(1-17)
CL                  C6      4(A17)
CL+                 C5     12(167)
CL+                 C6      6(237)
CL-                 B5     12(167)
CL-                 C5     12(167)
CL-                 C6     12(130)
CL  C5              G9     10( 19)
CL  F               C5     12(168)
CL  F               C6      1(133)
CL  F               C6      2(1-36)
CL  F               C6      4(A39)
CL  F               G2      1( 42)
CL  F               G9      2( 50)
CL  F    LI 2       A2      1( 61)
CL  F    LI 2       A2      1( 73)
CL  F    LI 2       A2      2( 99)
CL  F    LI 2       A2      2(105)
CL  F    LI 2       A5      4(C 2)
CL  F    MG         C6      2(1-52)
CL  F    MG         C6      4(A56)
CL  F    MG         G2      1( 43)
CL  F    MG         G9      2( 51)
CL  F    O   3      C5     12(168)
CL  F   3           B5     12(168)
CL  F   4H          C5     12(168)
CL  F   55          C5     12(174)
CL  H               A2      7( 90)
CL  H               C5     12(167)
CL  H               C6      2(1-34)
CL  H               C6      4(A37)
CL  H    MG   O     B2      1( 16)
CL  H    MG   O     B5      1( 17)
CL  H    MG   O     B5      2( 20)
CL  H    O          B5     12(168)
CL  H    O   2      B5     12(168)
CL  H    O   3      B5     12(168)
CL  H    O   4      A2      7( 94)
CL  H    O   4      B5     12(168)
CL  H   2LI(   O    B2      1( 21)
CL  H   2LI    O    B5      1( 22)
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O   2TI--O   2ZR    F2      5(158)
O   2TI--O   2ZR    F2      5(216)
O   2W              B2      6( 51)
O   2W              B2      8( 92)
O   2W              B3      8( 92)
O   2W              B5      8(102)
O   2W              B9      8(139)
O   2ZR             B2      5(179)
O   2ZR             B9      5(248)
O   2ZR             E2      5(160)
O   3               A2      7( 94)
O   3               C5     12(165)
O   3P -            B5     12(180)
O   3PB  SI         B2      8( 99)
O   3PB  SI         B3      8( 99)
O   3PB  SI         B5      8(102)
O   3PB  SI         B9      8(164)
O   3PB 2           B2      6( 52)
O   3PB 2           B2      8( 98)
O   3PB 2           B3      8( 98)
O   3PB 2           B5      8(102)
O   3PB 2           B9      8(162)
O   3S              B5     12(172)
O   3S              C5     12(172)
O   3S --           B5     12(172)
O   3S  2--         B5     12(172)
O   3SE             B5     12(174)
O   3SE--           B5     12(174)
O   3TE--           B5     12(175)
O   3TI 2           B2      5(176)
O   3TI 2           B9      5(233)
O   3W              B2      8( 92)
O   3W              B3      8( 92)
O   3W              B5      8(102)
O   3W              B9      8(141)
O   4P -3           B5     12(180)
O   4PB 2SI         B2      8( 99)
O   4PB 2SI         B3      8( 99)
O   4PB 2SI         B5      8(102)
O   4PB 2SI         B9      8(165)
O   4PB 3           B2      6( 52)
O   4PB 3           B2      8( 98)
O   4PB 3           B3      6( 52)
O   4PB 3           B3      8( 98)
O   4PB 3           B5      8(102)
O   4PB 3           B9      8(163)
O   4S --           B5     12(172)
O   4SF--           B5     12(174)
O   4SI  ZR         B2      7( 67)
O   5TI  O          B2      5(177)
O   5TI 3           B9      5(235)
O   6P  4           B5     12(180)
O   7P  2-4         B5     12(180)
O   8S  2--         B5     12(172)
O  10P  4           B5     12(180)
P                   B5     12(180)
P                   C6      2(1-15)
P                   C6      4(A15)
P +                 C6      6(233)
P   2               B5     12(180)
P   2S  3           B5     12(182)
P   4               B5     12(180)
PB                  B1      8( 96)
PB                  B2      6( 51)
PB                  B2      8( 96)
PB                  B3      6( 51)
PB                  B3      8( 96)
PB                  B5      8(102)
PB                  B9      8(156)
PB+                 C6      6(259)
S                   B5     12(171)
S                   C5     12(171)
S                   C6      2(1-16)
S                   C6      4(A16)
S  +                C5     12(171)
S  +                C6      6(235)
S  -                C5     12(171)
S  --               B5     12(171)
S   2               C5     12(171)
S   3               C5     12(171)
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CL  H  2LI  0       B5      2( 20)       S   4          C5      12(171)
CL  H  4N           B5     12(178)       S   5          C5      12(171)
CL  H  4N   0       B5     12(178)       S   6          C5      12(171)
CL  H  4N   0   4   A1      3( 53)       S   7          C5      12(171)
CL  H  4N   0   4   A1      4( 28)       S   8          C5      12(171)
CL  H  4N   0   4   A2      7( 94)       SE             B5      12(174)
CL  H  4N   0   4   B5     12(179)       SE  2          C5      12(174)
CL  H  5N  2        B5     12(178)       SE  6          C5      12(174)
CL  H  5N  20   4   A2      7( 94)       SI             B2       7( 68)
CL  H  5N  20   4   B5     12(179)       SI             B2      12( 98)
CL  HG              B2      9( 30)       SI             C6       2(1-14)
CL  HG              B9      9( 32)       SI             C6       4(A14)
CL  I               A2      7( 94)       SI+            C6       6(231)
CL  I               B5     12(171)       SI--TI         F2       5(202)
CL  I               C5     12(171)       SI--ZR         F2       5(203)
CL  K               A2      7( 90)       TE             B5      12(174)
CL  K               B2      7( 70)       TE  2          C5      12(175)
CL  K               B2     11( 91)       TI             A5       4(C 1)
CL  K               B3     11( 91)       TI             B2       3( 15)
CL  K               B9     11(173)       TI             B3       3( 15)
CL  K               G9     10( 19)       TI             B5       3( 16)
CL  K    0   3      B2      9( 26)       TI             B5       3( 21)
CL  K    0   3      B3     10( 40)       TI             B9       3( 22)
CL  K    0   3      B9      9( 32)       TI             B9       3(2-40)
CL  K    0   3      C5     12(184)       TI             B9       4(B40)
CL  K    0   4      A1      3( 53)       TI+            C6       6(245)
CL  K    0   4      A1      4( 28)       TI--B          F2       5(194)
CL  K    0   4      A2      7( 95)       TI--ZR         F2       5(204)
CL  K    0   4      A9      7( 10)       W              B2       6( 51)
CL  K    0   4      B1      7(  3)       W              B2       8( 91)
CL  K    0   4      B2      9( 26)       W              B3       6( 51)
CL  K    0   4      B3     10( 40)       W              B3       8( 91)
CL  K    0   4      B9      9( 32)       W              B5       8(102)
CL  K    0   4      B9     10( 74)       W              B9       8(137)
CL  K    0   4      C5     12(184)       W  +           C6       6(249)
CL  LI              A2      1( 61)       ZR             B1       5(180)
CL  LI              A2      1( 72)       ZR             B2       5(178)
CL  LI              A2      2( 99)       ZR             B2       5(180)
CL  LI              A2      2(105)       ZR             B9       5(241)
CL  LI              A5      4(C 2)       ZR             B9      11(154)
CL  LI              B1      1( 20)       ZR+            C6       6(251)
CL  LI              B1      2( 30)
CL  LI              B1      3( 63)
CL  LI              B1      5(176)
CL  LI              B2      1( 20)
CL  LI              B2      2( 30)
CL  LI              B2      3( 63)
CL  LI              B2      5(176)
CL  LI              B3      1( 27)
CL  LI              B5      1( 22)
CL  LI              B5      2( 20)
CL  LI              B9      2(2-26)
CL  LI              B9      4(B26)
CL  LI              B9      5(229)
CL  LI              C6      1(109)
CL  LI              C6      2(1-21)
CL  LI              C6      4(A21)
CL  LI              D2      2( 79)
CL  LI              G1     10( 13)
CL  LI              G1     10( 18)
CL  LI              G2      1( 42)
CL  LI              G9      2( 50)
CL  LI              G9     10( 18)
CL  LI              G9     10( 19)
CL  LI--F    LI     F2      5(163)
CL  LI--F    LI     F2      5(217)
CL  LI  0   4       A1      3( 53)
CL  LI  0   4       A1      4( 28)
CL  LI  0   4       A2      7( 95)
CL  MG              A2      1( 60)
CL  MG              A2      1( 70)
CL  MG              A2      2( 95)
CL  MG              A2      2(104)
CL  MG              A5      4(C 2)
CL  MG              C6      1(119)
CL  MG              C6      2(1-27)
CL  MG              C6      4(A27)
CL  MG              G2      1( 42)
CL  MG              G9      2( 50)
CL  N    0          A2      7( 94)
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APPENDIX II

THERMODYNAMIC FUNCTIONS OF SOME SELECTED SUBSTANCES IN THE SOLID AND LIQUID STATES

George T. Furukawa and Martin L. Reilly

The low-temperature heat-capacity and the high-temperature relative-enthalpy data on some selected substances that should be of interest to the light-element thermodynamics program were analyzed. Sources of literature data that were compiled for the analysis have been given for most of the substances in a previous report of this series [1]. The low-temperature heat-capacity data were examined and selected for general consistency and joined smoothly with the values of heat capacity at the high temperatures calculated from the enthalpy equations reported by the original investigators or given by Kelley [2]. Where the lower temperature limit of the data was fairly high (e.g. about 50°K), the equation selected by the original investigator was used for extrapolation to 0°K and joined smoothly with the experimental data. The thermodynamic functions were calculated from the smoothed tabular values of heat capacity by numerical integration using the 4-point Lagrangian integration coefficient method [3] in conjunction with the usual thermodynamic relations. Sources of data actually used in obtaining the thermodynamic functions are given along with each of the tables.

The 1961 atomic weights based on C-12 [4] and the energy relation: 4.1840 joules = 1 defined calorie, were used in calculating the gram molal thermodynamic functions given in the tables.

References

[1] "Preliminary Report on the Thermodynamic Properties of Selected Light-Element and Some Related Compounds", National Bureau of Standards, Washington, D. C., 20234. NBS Report 8504, 1 July 1964, p 86.

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

[3] "Tables of Lagrangian Interpolation Coefficients" Columbia University Press, New York, 1944.

[4] "IUPAC Revises Atomic Weight Values", Chem. Eng. News 39, 42 (1961).

TABLE B-116

THERMODYNAMIC FUNCTIONS FOR CRYOLITE ($NA_3AL F_6$)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.= 209.9413 GRAMS CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

SOLID PHASE (ALPHA)

T DEG K	$-(G_T^0-H_0^0)/T$ CAL/DEG MOLE	$(H_T^0-H_0^0)/T$ CAL/DEG MOLE	$(S_T-S_0^0)$ CAL/DEG MOLE	$(H_T^0-H_0^0)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.002	0.005	0.006	0.024	0.019	0.008
10.00	0.013	0.039	0.052	0.389	0.155	0.130
15.00	0.043	0.129	0.172	1.931	0.502	0.652
20.00	0.101	0.290	0.391	5.810	1.088	2.018
25.00	0.190	0.527	0.717	13.170	1.893	4.743
30.00	0.312	0.837	1.149	25.109	2.920	9.361
35.00	0.469	1.222	1.691	42.771	4.179	16.416
40.00	0.661	1.680	2.341	67.211	5.621	26.454
45.00	0.889	2.203	3.092	99.156	7.171	39.999
50.00	1.150	2.780	3.931	139.01	8.777	57.522
55.00	1.444	3.399	4.843	186.95	10.403	79.428
60.00	1.768	4.051	5.818	243.04	12.032	106.06
65.00	2.118	4.727	6.845	307.26	13.654	137.70
70.00	2.494	5.422	7.916	379.54	15.253	174.58
75.00	2.892	6.130	9.022	459.72	16.811	216.92
80.00	3.311	6.844	10.155	547.56	18.314	264.85
85.00	3.747	7.562	11.309	642.77	19.762	318.50
90.00	4.200	8.279	12.478	745.10	21.166	377.96
95.00	4.666	8.993	13.660	854.38	22.538	443.30
100.00	5.146	9.704	14.850	970.43	23.879	514.58
105.00	5.636	10.411	16.047	1093.1	25.187	591.82
110.00	6.137	11.111	17.248	1222.2	26.456	675.05
115.00	6.646	11.805	18.451	1357.6	27.684	764.30
120.00	7.163	12.492	19.655	1499.0	28.870	859.56
125.00	7.687	13.170	20.857	1646.2	30.016	960.84
130.00	8.216	13.839	22.056	1799.1	31.126	1068.1
135.00	8.751	14.499	23.251	1957.4	32.199	1181.4
140.00	9.290	15.150	24.440	2121.0	33.236	1300.6
145.00	9.833	15.791	25.624	2289.7	34.232	1425.8
150.00	10.379	16.422	26.801	2463.3	35.187	1556.9
155.00	10.928	17.042	27.970	2641.5	36.100	1693.8
160.00	11.478	17.651	29.130	2824.2	36.971	1836.5
165.00	12.031	18.250	30.280	3011.2	37.803	1985.1
170.00	12.584	18.836	31.421	3202.2	38.600	2139.3
175.00	13.139	19.412	32.551	3397.1	39.365	2299.3
180.00	13.693	19.977	33.670	3595.8	40.101	2464.8
185.00	14.248	20.530	34.778	3798.1	40.809	2635.9
190.00	14.803	21.073	35.876	4003.8	41.492	2812.6
195.00	15.357	21.605	36.962	4213.0	42.149	2994.7
200.00	15.911	22.126	38.037	4425.3	42.783	3182.2
205.00	16.464	22.638	39.101	4640.7	43.393	3375.0
210.00	17.015	23.139	40.154	4859.2	43.980	3573.2
215.00	17.565	23.630	41.196	5080.5	44.545	3776.6
220.00	18.114	24.112	42.226	5304.6	45.090	3985.1
225.00	18.661	24.584	43.245	5531.4	45.615	4198.8
230.00	19.207	25.047	44.253	5760.7	46.122	4417.5
235.00	19.750	25.500	45.251	5992.6	46.612	4641.3
240.00	20.292	25.945	46.237	6226.8	47.086	4870.0
245.00	20.831	26.381	47.212	6463.4	47.545	5103.7
250.00	21.369	26.809	48.178	6702.2	47.988	5342.1
255.00	21.904	27.228	49.132	6943.3	48.417	5585.4
260.00	22.436	27.640	50.076	7186.4	48.832	5833.4
265.00	22.967	28.044	51.010	7431.5	49.231	6086.2
270.00	23.495	28.440	51.934	7678.7	49.615	6343.5
273.15	23.826	28.685	52.511	7835.3	49.850	6508.0
275.00	24.020	28.828	52.848	7927.7	49.984	6605.5
280.00	24.543	29.209	53.752	8178.5	50.338	6872.0
285.00	25.063	29.583	54.646	8431.0	50.676	7143.0
290.00	25.581	29.949	55.530	8685.2	50.999	7418.4
295.00	26.096	30.308	56.404	8941.0	51.308	7698.3
298.15	26.419	30.531	56.950	9102.9	51.495	7876.8
300.00	26.608	30.661	57.269	9198.3	51.603	7982.5

TABLE B-116 (CONT.)

THERMODYNAMIC FUNCTIONS FOR CRYOLITE ($NA_3AL\ F_6$)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.= 209.9413 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^C_0)/T$ CAL/DEG MOLE	$(H^0_T-H^C_0)/T$ CAL/DEG MOLE	$(S_T-S^C_0)$ CAL/DEG MOLE	$(H^0_T-H^C_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^C_0)$ CAL/MOLE
SOLID PHASE (ALPHA)						
300.00	26.608	30.661	57.269	9198.3	51.603	7982.5
310.00	27.625	31.345	58.970	9717.1	52.154	8563.7
320.00	28.630	32.004	60.634	10241.	52.662	9161.7
330.00	29.625	32.637	62.262	10770.	53.135	9776.2
340.00	30.608	33.247	63.855	11304.	53.581	10407.
350.00	31.581	33.834	65.414	11842.	54.009	11053.
360.00	32.542	34.400	66.942	12384.	54.423	11715.
370.00	33.492	34.946	68.438	12930.	54.826	12392.
373.15	33.789	35.115	68.904	13103.	54.952	12608.
380.00	34.431	35.475	69.905	13480.	55.223	13084.
390.00	35.359	35.986	71.345	14035.	55.612	13790.
400.00	36.276	36.482	72.758	14593.	55.995	14511.
425.00	38.524	37.657	76.181	16004.	56.930	16373.
450.00	40.707	38.753	79.461	17439.	57.833	18318.
475.00	42.831	39.781	82.611	18896.	58.711	20345.
500.00	44.896	40.749	85.644	20374.	59.568	22448.
550.00	48.865	42.535	91.400	23395.	61.233	26876.
600.00	52.637	44.161	96.798	26497.	62.853	31582.
650.00	56.231	45.660	101.89	29679.	64.440	36550.
700.00	59.667	47.058	106.72	32940.	66.004	41767.
750.00	62.959	48.372	111.33	36279.	67.550	47219.
800.00	66.121	49.619	115.74	39695.	69.084	52897.
845.00	68.865	50.692	119.56	42835.	70.454	58191.
SOLID PHASE (BETA)						
845.00	68.865	53.248	122.11	44995.	65.552	58191.
850.00	69.179	53.321	122.50	45323.	65.631	58803.
900.00	72.247	54.027	126.27	48624.	66.424	65023.
950.00	75.167	54.700	129.89	51965.	67.217	71427.
1000.00	78.009	55.346	133.35	55346.	68.010	78009.
1050.00	80.724	55.968	136.69	58766.	68.803	84761.
1100.00	83.342	56.569	139.91	62226.	69.596	91676.
1150.00	85.869	57.153	143.02	65726.	70.389	98750.
1200.00	88.314	57.721	146.03	69265.	71.182	105977.
1250.00	90.681	58.275	148.96	72844.	71.975	113352.
1300.00	92.978	58.817	151.79	76462.	72.768	120871.
LIQUID PHASE						
1300.00	92.978	80.079	173.06	104102.	93.400	120871.
1350.00	96.009	80.572	176.58	108772.	93.400	129612.
1400.00	98.948	81.030	179.98	113442.	93.400	138527.
1450.00	101.80	81.457	183.26	118112.	93.400	147608.
1500.00	104.57	81.855	186.42	122782.	93.400	156851.

H^C_0 AND S^C_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

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Cryolite, Anhydrous Aluminum Fluoride and Sodium Fluoride
J. Am. Chem. Soc. 79, 2056-2057 (1957)

Kelley, K. K.,
Contributions to the Data on Theoretical Metallurgy.
XIII. High-Temperature Heat-Content, Heat-Capacity,
and Entropy Data for the Elements and Inorganic Compounds
U. S. Bur. Mines, Bull. 584, 232 pages (1960)

TABLE B-117

THERMODYNAMIC FUNCTIONS FOR SODIUM ORTHOSILICATE ($NA_4SI\ O_4$)
SOLID PHASE

GRAM MOLECULAR WT.= 184.0428 GRAMS CAL=4.1840 ABS J
T OEG K = 273.15 + T OEG C

T OEG K	$-(G_T^0-H_0^C)/T$ CAL / OEG MOLE	$(H_T^0-H_0^C)/T$ CAL / OEG MOLE	$(S_T-S_0^C)$ CAL / OEG MOLE	$(H_T^0-H_0^C)$ CAL / MOLE	C_P^0 CAL / OEG MOLE	$-(G_T^0-H_0^C)$ CAL / MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.002	0.006	0.005	0.002
10.00	0.003	0.010	0.013	0.099	0.040	0.033
15.00	0.011	0.034	0.045	0.503	0.134	0.167
20.00	0.027	0.080	0.107	1.302	0.326	0.530
25.00	0.052	0.161	0.213	4.024	0.677	1.308
30.00	0.092	0.293	0.385	8.785	1.276	2.772
35.00	0.152	0.494	0.646	17.299	2.178	5.309
40.00	0.235	0.776	1.011	31.052	3.364	9.407
45.00	0.347	1.140	1.486	51.282	4.754	15.607
50.00	0.489	1.576	2.064	78.775	6.258	24.442
55.00	0.662	2.073	2.734	113.99	7.835	36.401
60.00	0.865	2.619	3.484	157.16	9.433	51.917
65.00	1.098	3.204	4.302	208.26	11.002	71.357
70.00	1.357	3.816	5.173	267.11	12.527	95.024
75.00	1.642	4.446	6.088	333.44	13.997	123.16
80.00	1.949	5.087	7.036	406.97	15.401	155.96
85.00	2.277	5.733	8.010	487.33	16.732	193.57
90.00	2.623	6.380	9.003	574.18	17.998	236.09
95.00	2.985	7.023	10.009	667.22	19.209	283.62
100.00	3.362	7.662	11.024	766.20	20.377	336.20
105.00	3.751	8.295	12.046	870.93	21.510	393.87
110.00	4.151	8.920	13.072	981.23	22.607	456.66
115.00	4.562	9.539	14.100	1096.9	23.667	524.59
120.00	4.981	10.149	15.129	1217.8	24.683	597.66
125.00	5.407	10.749	16.156	1343.7	25.652	675.88
130.00	5.840	11.341	17.181	1474.3	26.573	759.22
135.00	6.279	11.921	18.200	1609.3	27.446	847.67
140.00	6.723	12.490	19.213	1748.7	28.276	941.21
145.00	7.171	13.049	20.219	1892.0	29.069	1039.8
150.00	7.623	13.595	21.218	2039.3	29.830	1143.4
155.00	8.077	14.131	22.208	2190.3	30.564	1252.0
160.00	8.534	14.656	23.190	2344.9	31.277	1365.5
165.00	8.993	15.170	24.163	2503.0	31.969	1483.8
170.00	9.453	15.674	25.127	2664.6	32.641	1607.1
175.00	9.915	16.168	26.083	2829.4	33.292	1735.1
180.00	10.377	16.652	27.030	2997.4	33.920	1867.9
185.00	10.840	17.127	27.967	3168.6	34.522	2005.4
190.00	11.303	17.593	28.896	3342.6	35.100	2147.5
195.00	11.766	18.049	29.814	3519.5	35.653	2294.3
200.00	12.228	18.496	30.724	3699.1	36.183	2445.7
205.00	12.690	18.933	31.624	3881.3	36.693	2601.5
210.00	13.152	19.362	32.514	4066.0	37.187	2761.9
215.00	13.612	19.782	33.394	4253.2	37.665	2926.7
220.00	14.072	20.194	34.266	4442.6	38.131	3095.8
225.00	14.530	20.598	35.128	4634.4	38.586	3269.3
230.00	14.987	20.993	35.981	4828.5	39.030	3447.1
235.00	15.443	21.382	36.825	5024.7	39.463	3629.1
240.00	15.897	21.763	37.660	5223.1	39.885	3815.3
245.00	16.350	22.137	38.487	5423.6	40.295	4005.7
250.00	16.801	22.504	39.305	5626.0	40.692	4200.2
255.00	17.250	22.865	40.114	5830.5	41.076	4398.7
260.00	17.697	23.218	40.916	6036.8	41.445	4601.3
265.00	18.143	23.566	41.708	6244.9	41.801	4807.9
270.00	18.587	23.906	42.493	6454.8	42.141	5018.4
273.15	18.865	24.118	42.983	6587.8	42.349	5153.0
275.00	19.028	24.241	43.269	6666.3	42.468	5232.8
280.00	19.468	24.569	44.037	6879.4	42.780	5451.0
285.00	19.906	24.891	44.797	7094.1	43.078	5673.1
290.00	20.341	25.207	45.549	7310.2	43.362	5899.0
295.00	20.775	25.517	46.292	7527.7	43.633	6128.6
298.15	21.047	25.712	46.759	7665.4	43.796	6275.2
300.00	21.206	25.822	47.028	7746.5	43.890	6361.9

H_0^C ANO S_0^C APPLY TO THE REFERENCE STATE OF THE SOLIO AT ZERO OEG K

Kelley, K. K.,
The Specific Heats at Low Temperatures of Crystalline
Ortho-, Meta-, andDi- silicates of Sodium
J. Am. Chem. Soc. 61, 471-473 (1939)

TABLE B-118

THERMODYNAMIC FUNCTIONS FOR BARIUM OXIDE (8A O)
SOLID PHASE

GRAM MOLECULAR WT.= 153.3394 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T OEG C

T DEG K	$-(G_T^0-H_0^C)/T$ CAL/DEG MOLE	$(H_T^0-H_0^C)/T$ CAL/OEG MOLE	$(S_T-S_0^C)$ CAL/DEG MOLE	$(H_T^0-H_0^C)$ CAL/MOLE	C_P^0 CAL/OEG MOLE	$-(G_T^0-H_0^C)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.003	0.004	0.014	0.011	0.005
10.00	0.007	0.022	0.030	0.225	0.090	0.075
15.00	0.025	0.075	0.101	1.132	0.299	0.378
20.00	0.059	0.175	0.234	3.492	0.671	1.186
25.00	0.113	0.322	0.435	8.054	1.169	2.832
30.00	0.188	0.509	0.697	15.272	1.721	5.642
35.00	0.282	0.722	1.004	25.269	2.277	9.879
40.00	0.393	0.950	1.344	38.017	2.819	15.738
45.00	0.519	1.187	1.706	53.433	3.344	23.355
50.00	0.657	1.429	2.086	71.443	3.858	32.830
55.00	0.804	1.673	2.477	91.989	4.358	44.231
60.00	0.960	1.917	2.877	114.99	4.841	57.612
65.00	1.123	2.159	3.283	140.36	5.299	73.009
70.00	1.292	2.399	3.691	167.93	5.726	90.443
75.00	1.466	2.634	4.100	197.55	6.113	109.92
80.00	1.643	2.863	4.506	229.00	6.464	131.43
85.00	1.823	3.084	4.907	262.13	6.784	154.97
90.00	2.005	3.298	5.303	296.81	7.083	180.50
95.00	2.189	3.505	5.694	332.93	7.365	207.99
100.00	2.374	3.704	6.079	370.43	7.633	237.43
105.00	2.560	3.898	6.457	409.24	7.888	268.77
110.00	2.745	4.084	6.830	449.29	8.128	301.99
115.00	2.931	4.265	7.196	490.49	8.352	337.06
120.00	3.116	4.440	7.556	532.78	8.559	373.94
125.00	3.301	4.608	7.909	576.06	8.750	412.61
130.00	3.485	4.771	8.256	620.25	8.925	453.02
135.00	3.668	4.928	8.596	665.29	9.088	495.15
140.00	3.850	5.079	8.929	711.11	9.239	538.97
145.00	4.031	5.225	9.256	757.66	9.380	584.44
150.00	4.210	5.366	9.576	804.89	9.511	631.52
155.00	4.388	5.502	9.890	852.75	9.634	680.19
160.00	4.565	5.633	10.198	901.22	9.749	730.41
165.00	4.740	5.759	10.499	950.23	9.857	782.15
170.00	4.914	5.881	10.795	999.77	9.957	835.39
175.00	5.086	5.999	11.085	1049.8	10.052	890.09
180.00	5.257	6.113	11.370	1100.3	10.141	946.23
185.00	5.426	6.223	11.649	1151.2	10.225	1003.8
190.00	5.593	6.329	11.922	1202.5	10.306	1062.7
195.00	5.759	6.432	12.191	1254.2	10.382	1123.0
200.00	5.923	6.532	12.455	1306.3	10.455	1184.6
205.00	6.086	6.628	12.714	1358.8	10.524	1247.5
210.00	6.246	6.722	12.968	1411.6	10.590	1311.7
215.00	6.406	6.812	13.218	1464.7	10.654	1377.2
220.00	6.563	6.900	13.464	1518.1	10.714	1443.9
225.00	6.719	6.986	13.705	1571.8	10.772	1511.8
230.00	6.874	7.069	13.943	1625.8	10.828	1581.0
235.00	7.027	7.149	14.176	1680.1	10.881	1651.3
240.00	7.178	7.228	14.406	1734.6	10.932	1722.7
245.00	7.328	7.304	14.632	1789.4	10.981	1795.3
250.00	7.476	7.378	14.854	1844.4	11.028	1869.0
255.00	7.623	7.450	15.073	1899.7	11.074	1943.8
260.00	7.768	7.520	15.288	1955.2	11.118	2019.7
265.00	7.912	7.588	15.500	2010.9	11.161	2096.7
270.00	8.055	7.655	15.709	2066.8	11.202	2174.7
273.15	8.144	7.696	15.839	2102.1	11.228	2224.4
275.00	8.196	7.720	15.915	2122.9	11.242	2253.8
280.00	8.335	7.783	16.118	2179.2	11.282	2333.9
285.00	8.474	7.845	16.318	2235.7	11.319	2415.0
290.00	8.611	7.905	16.515	2292.4	11.356	2497.1
295.00	8.746	7.964	16.710	2349.3	11.392	2580.1
298.15	8.831	8.000	16.831	2385.2	11.415	2633.0
300.00	8.881	8.021	16.902	2406.3	11.427	2664.2

TABLE B-118 (CONT.)

THERMODYNAMIC FUNCTIONS FOR BARIUM OXIDE (BA O)
SOLID PHASE

GRAM MOLECULAR WT.= 153.3394 GRAMS   CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^C)/T$ CAL / DEG MOLE	$(H_T^0-H_0^C)/T$ CAL / DEG MOLE	$(S_T-S_0^C)$ CAL / DEG MOLE	$(H_T^0-H_0^C)$ CAL / MOLE	C_P^0 CAL / DEG MOLE	$-(G_T^0-H_0^C)$ CAL / MOLE
300.00	8.881	8.021	16.902	2406.3	11.427	2664.2
310.00	9.145	8.132	17.277	2520.9	11.495	2835.1
320.00	9.405	8.238	17.643	2636.2	11.560	3009.7
330.00	9.660	8.340	18.000	2752.1	11.621	3187.9
340.00	9.911	8.437	18.348	2868.6	11.680	3369.7
350.00	10.157	8.531	18.687	2985.7	11.737	3554.8
360.00	10.398	8.620	19.019	3103.4	11.792	3743.4
370.00	10.636	8.707	19.343	3221.6	11.845	3935.2
373.15	10.710	8.733	19.443	3258.9	11.861	3996.3
380.00	10.869	8.790	19.659	3340.3	11.895	4130.2
390.00	11.098	8.870	19.969	3459.5	11.944	4328.3
400.00	11.324	8.948	20.272	3579.1	11.991	4529.6
425.00	11.872	9.130	21.002	3880.3	12.101	5045.6
450.00	12.399	9.298	21.697	4184.1	12.201	5579.4
475.00	12.905	9.453	22.359	4490.3	12.293	6130.1
500.00	13.394	9.597	22.992	4798.7	12.378	6697.0
550.00	14.321	9.857	24.179	5421.6	12.533	7876.7
600.00	15.189	10.086	25.275	6051.8	12.674	9113.4
650.00	16.005	10.290	26.295	6688.7	12.804	10403.
700.00	16.774	10.474	27.248	7332.0	12.926	11742.
750.00	17.502	10.642	28.144	7981.3	13.044	13127.
800.00	18.194	10.795	28.990	8636.3	13.157	14555.
850.00	18.853	10.938	29.791	9296.9	13.266	16025.
900.00	19.482	11.070	30.552	9962.9	13.373	17534.
950.00	20.084	11.194	31.278	10634.	13.479	19080.
1000.00	20.661	11.311	31.972	11311.	13.582	20661.
1050.00	21.216	11.421	32.637	11992.	13.684	22276.
1100.00	21.749	11.526	33.276	12679.	13.785	23924.
1150.00	22.264	11.627	33.891	13371.	13.886	25603.
1200.00	22.761	11.723	34.484	14068.	13.985	27313.
1250.00	23.241	11.816	35.057	14769.	14.084	29052.
1300.00	23.706	11.905	35.611	15476.	14.182	30818.
1350.00	24.157	11.991	36.148	16188.	14.280	32612.
1400.00	24.595	12.074	36.669	16904.	14.377	34433.
1450.00	25.020	12.155	37.175	17625.	14.474	36279.
1500.00	25.434	12.234	37.668	18351.	14.571	38150.
1550.00	25.836	12.311	38.147	19082.	14.667	40046.
1600.00	26.228	12.386	38.614	19818.	14.764	41965.
1650.00	26.610	12.460	39.070	20558.	14.860	43907.
1700.00	26.983	12.532	39.515	21304.	14.955	45872.
1750.00	27.343	12.602	39.950	22054.	15.051	47858.
1800.00	27.704	12.672	40.375	22809.	15.147	49866.
1850.00	28.052	12.740	40.791	23569.	15.242	51896.
1900.00	28.392	12.807	41.199	24333.	15.338	53945.
1950.00	28.726	12.873	41.599	25102.	15.433	56015.
2000.00	29.053	12.938	41.991	25876.	15.528	58105.

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

Anderson, C. T.,
The Heat Capacities at Low Temperatures of the Oxides of
Strontium and Barium
J. Am. Chem. Soc. 57, 429-431 (1935)

Kelley, K. K.,
Contributions to the Data on Theoretical Metallurgy.
XIII. High-Temperature Heat-Content, Heat-Capacity,
and Entropy Data for the Elements and Inorganic Compounds
U. S. Bur. Mines, Bull. 584, 232 pages (1960)

TABLE B-119

THERMODYNAMIC FUNCTIONS FOR CALCIUM CARBIDE ($CA\ C_2$)
SOLID PHASES

GRAM MOLECULAR WT.= 64.1023 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T	$-(G^0_T-H^C_0)/T$	$(H^0_T-H^C_0)/T$	$(S_T-S^C_0)$	$(H^0_T-H^C_0)$	C^0_P	$-(G^0_T-H^C_0)$
DEG K	CAL/DEG MOLE	CAL/DEG MOLE	CAL/DEG MOLE	CAL/MOLE	CAL/DEG MOLE	CAL/MOLE
			SOLID PHASE (ALPHA)			
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.001	0.004	0.003	0.001
10.00	0.002	0.006	0.008	0.056	0.023	0.019
15.00	0.007	0.020	0.027	0.303	0.083	0.099
20.00	0.016	0.049	0.065	0.973	0.195	0.318
25.00	0.031	0.095	0.126	2.377	0.379	0.784
30.00	0.054	0.163	0.218	4.899	0.643	1.632
35.00	0.086	0.255	0.342	8.939	0.984	3.016
40.00	0.128	0.371	0.499	14.844	1.386	5.103
45.00	0.179	0.508	0.687	22.865	1.827	8.055
50.00	0.240	0.663	0.903	33.138	2.295	12.019
55.00	0.311	0.831	1.143	45.728	2.754	17.125
60.00	0.391	1.012	1.403	60.722	3.247	23.482
65.00	0.480	1.204	1.684	78.241	3.764	31.191
70.00	0.576	1.405	1.982	98.373	4.289	40.347
75.00	0.680	1.615	2.295	121.13	4.811	51.034
80.00	0.792	1.831	2.622	146.46	5.323	63.324
85.00	0.909	2.051	2.960	174.34	5.825	77.276
90.00	1.033	2.274	3.307	204.69	6.313	92.940
95.00	1.162	2.499	3.661	237.44	6.786	110.36
100.00	1.296	2.725	4.021	272.52	7.242	129.56
105.00	1.434	2.951	4.385	309.84	7.683	150.57
110.00	1.576	3.176	4.752	349.32	8.108	173.41
115.00	1.723	3.399	5.122	390.89	8.517	198.10
120.00	1.872	3.621	5.493	434.47	8.910	224.63
125.00	2.024	3.840	5.864	479.96	9.284	253.02
130.00	2.179	4.056	6.235	527.27	9.635	283.27
135.00	2.336	4.269	6.605	576.27	9.963	315.37
140.00	2.495	4.478	6.973	626.87	10.270	349.32
145.00	2.656	4.682	7.338	678.94	10.558	385.09
150.00	2.818	4.883	7.701	732.42	10.829	422.69
155.00	2.981	5.079	8.060	787.22	11.088	462.10
160.00	3.146	5.270	8.416	843.28	11.335	503.29
165.00	3.311	5.458	8.768	900.95	11.571	546.25
170.00	3.476	5.641	9.117	958.97	11.798	590.97
175.00	3.642	5.820	9.462	1018.5	12.012	637.42
180.00	3.809	5.995	9.804	1079.1	12.216	685.58
185.00	3.975	6.166	10.141	1140.6	12.407	735.45
190.00	4.142	6.332	10.474	1203.1	12.586	786.99
195.00	4.309	6.495	10.803	1266.5	12.754	840.18
200.00	4.475	6.653	11.128	1330.6	12.912	895.01
205.00	4.641	6.808	11.449	1395.6	13.060	951.46
210.00	4.807	6.958	11.765	1461.2	13.201	1009.5
215.00	4.973	7.105	12.078	1527.6	13.334	1069.1
220.00	5.138	7.248	12.386	1594.6	13.461	1130.3
225.00	5.302	7.387	12.689	1662.2	13.583	1193.0
230.00	5.466	7.523	12.989	1730.4	13.700	1257.2
235.00	5.629	7.656	13.285	1799.2	13.813	1322.8
240.00	5.792	7.785	13.577	1868.5	13.923	1390.0
245.00	5.953	7.912	13.865	1938.4	14.029	1458.6
250.00	6.115	8.035	14.150	2008.8	14.133	1528.6
255.00	6.275	8.156	14.431	2079.7	14.233	1600.1
260.00	6.434	8.274	14.708	2151.1	14.331	1672.9
265.00	6.593	8.389	14.982	2223.0	14.426	1747.2
270.00	6.751	8.501	15.252	2295.4	14.518	1822.8
273.15	6.850	8.571	15.421	2341.2	14.575	1871.1
275.00	6.908	8.612	15.520	2368.2	14.608	1899.7
280.00	7.064	8.719	15.784	2441.5	14.696	1978.0
285.00	7.219	8.825	16.044	2515.2	14.781	2057.5
290.00	7.374	8.929	16.302	2589.3	14.864	2138.4
295.00	7.527	9.030	16.557	2663.8	14.944	2220.5
298.15	7.623	9.093	16.716	2710.9	14.994	2272.9
300.00	7.680	9.129	16.809	2738.7	15.023	2304.0

TABLE B-119 (CONT.)

THERMODYNAMIC FUNCTIONS FOR CALCIUM CARBIDE (CA C_2)
SOLID PHASES

GRAM MOLECULAR WT.= 64.1023 GRAMS   CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T	$-(G^0_T-H^C_0)/T$	$(H^0_T-H^C_0)/T$	$S_T-S^C_0$	$(H^0_T-H^C_0)$	C^0_p	$-(G^0_T-H^C_0)$
DEG K	CAL / DEG MOLE	CAL / DEG MOLE	CAL / DEG MOLE	CAL / MOLE	CAL / DEG MOLE	CAL / MOLE
			SOLID PHASE (ALPHA)			
300.00	7.680	9.129	16.809	2738.7	15.023	2304.0
310.00	7.982	9.322	17.304	2889.7	15.173	2474.5
320.00	8.281	9.507	17.788	3042.2	15.317	2650.0
330.00	8.577	9.685	18.261	3196.0	15.453	2830.3
340.00	8.868	9.856	18.725	3351.2	15.582	3015.2
350.00	9.156	10.022	19.178	3507.6	15.706	3204.7
360.00	9.441	10.181	19.622	3665.3	15.824	3398.7
370.00	9.722	10.335	20.057	3824.1	15.936	3597.1
373.15	9.810	10.383	20.193	3874.3	15.971	3660.5
380.00	10.000	10.484	20.484	3984.0	16.043	3799.8
390.00	10.274	10.628	20.902	4144.9	16.145	4006.8
400.00	10.545	10.767	21.312	4306.9	16.241	4217.8
425.00	11.207	11.096	22.303	4715.7	16.461	4763.1
450.00	11.850	11.399	23.250	5129.7	16.656	5332.6
475.00	12.474	11.681	24.155	5548.3	16.832	5925.3
500.00	13.080	11.942	25.022	5971.2	16.992	6540.1
550.00	14.241	12.415	26.656	6828.1	17.278	7832.5
600.00	15.339	12.831	28.170	7698.4	17.529	9203.6
650.00	16.381	13.201	29.582	8580.6	17.756	10648.
700.00	17.372	13.534	30.906	9473.7	17.966	12160.
720.00	17.755	13.658	31.413	9833.8	18.045	12784.
			SOLID PHASE (BETA)			
720.00	17.755	15.505	33.260	11164.	16.840	12783.
750.00	18.389	15.560	33.949	11670.	16.900	13792.
800.00	19.396	15.647	35.043	12517.	17.000	15517.
850.00	20.347	15.729	36.076	13370.	17.100	17295.
900.00	21.248	15.808	37.057	14227.	17.200	19124.
950.00	22.105	15.884	37.989	15090.	17.300	21000.
1000.00	22.922	15.957	38.879	15957.	17.400	22922.
1050.00	23.702	16.029	39.731	16830.	17.500	24887.
1100.00	24.449	16.098	40.547	17707.	17.600	26894.
1150.00	25.166	16.165	41.332	18590.	17.700	28941.
1200.00	25.856	16.231	42.087	19477.	17.800	31027.
1250.00	26.520	16.296	42.816	20370.	17.900	33150.
1300.00	27.160	16.360	43.520	21267.	18.000	35308.
1350.00	27.779	16.422	44.201	22170.	18.100	37501.
1400.00	28.377	16.484	44.861	23077.	18.200	39728.
1450.00	28.957	16.545	45.501	23990.	18.300	41987.
1500.00	29.518	16.605	46.123	24907.	18.400	44278.

H^C_0 AND S^C_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

Kelley, K. K.,
Specific Heat of Calcium Carbide at Low Temperatures
Ind. Eng. Chem. 33, No. 10, 1314-1315 (1941)

Kelley, K. K.,
Contributions to the Data on Theoretical Metallurgy.
XIII. High-Temperature Heat-Content, Heat-Capacity,
and Entropy Data for the Elements and Inorganic Compounds
U. S. Bur. Mines, Bull. 584, 232 pages (1960)

TABLE B-120

THERMODYNAMIC FUNCTIONS FOR TRICALCIUM ALUMINATE ($3CA\ O\ .AL_2O_3$)
SOLID PHASE

GRAM MOLECULAR WT.= 270.1994 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^C_0)/T$ CAL/DEG MOLE	$(H^0_T-H^C_0)/T$ CAL/DEG MOLE	$(S_T-S^C_0)$ CAL/DEG MOLE	$(H^0_T-H^C_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^C_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.003	0.004	0.016	0.013	0.005
10.00	0.009	0.026	0.035	0.259	0.104	0.086
15.00	0.029	0.087	0.116	1.302	0.343	0.436
20.00	0.068	0.200	0.268	3.998	0.765	1.364
25.00	0.130	0.368	0.497	9.191	1.332	3.246
30.00	0.215	0.584	0.799	17.506	2.010	6.458
35.00	0.324	0.843	1.167	29.497	2.803	11.345
40.00	0.456	1.146	1.602	45.827	3.747	18.239
45.00	0.611	1.493	2.104	67.205	4.825	27.475
50.00	0.788	1.886	2.673	94.279	6.021	39.391
55.00	0.988	2.319	3.306	127.53	7.289	54.315
60.00	1.209	2.787	3.996	167.24	8.600	72.549
65.00	1.452	3.286	4.738	213.59	9.946	94.364
70.00	1.714	3.810	5.525	266.73	11.311	120.00
75.00	1.996	4.356	6.352	326.71	12.680	149.68
80.00	2.295	4.919	7.214	393.52	14.045	183.58
85.00	2.610	5.496	8.106	467.14	15.401	221.87
90.00	2.941	6.083	9.024	547.51	16.744	264.68
95.00	3.286	6.680	9.965	634.55	18.071	312.15
100.00	3.644	7.282	10.926	728.20	19.383	364.37
105.00	4.014	7.889	11.903	828.35	20.677	421.43
110.00	4.395	8.499	12.894	934.93	21.948	483.42
115.00	4.786	9.111	13.897	1047.8	23.192	550.39
120.00	5.187	9.723	14.910	1166.8	24.402	622.40
125.00	5.596	10.334	15.930	1291.6	25.570	699.50
130.00	6.013	10.942	16.955	1422.5	26.714	781.71
135.00	6.437	11.547	17.984	1558.8	27.816	869.06
140.00	6.868	12.147	19.015	1700.6	28.886	961.56
145.00	7.305	12.742	20.047	1847.6	29.924	1059.2
150.00	7.747	13.332	21.079	1999.8	30.933	1162.0
155.00	8.194	13.916	22.109	2156.9	31.912	1270.0
160.00	8.645	14.493	23.137	2318.9	32.860	1383.1
165.00	9.099	15.063	24.163	2485.5	33.779	1501.4
170.00	9.557	15.627	25.184	2656.6	34.666	1624.7
175.00	10.018	16.183	26.202	2832.1	35.524	1753.2
180.00	10.482	16.732	27.214	3011.8	36.352	1886.7
185.00	10.948	17.273	28.221	3195.6	37.153	2025.3
190.00	11.416	17.807	29.222	3383.3	37.928	2168.9
195.00	11.885	18.332	30.217	3574.8	38.679	2317.6
200.00	12.356	18.850	31.206	3770.0	39.407	2471.1
205.00	12.827	19.360	32.187	3968.8	40.115	2629.6
210.00	13.300	19.863	33.162	4171.1	40.803	2793.0
215.00	13.773	20.357	34.130	4376.8	41.472	2961.2
220.00	14.247	20.845	35.091	4585.8	42.123	3134.3
225.00	14.720	21.325	36.045	4798.0	42.755	3312.1
230.00	15.194	21.797	36.992	5013.3	43.371	3494.7
235.00	15.668	22.263	37.931	5231.7	43.968	3682.0
240.00	16.142	22.721	38.862	5453.0	44.549	3874.0
245.00	16.615	23.172	39.787	5677.2	45.112	4070.6
250.00	17.087	23.616	40.704	5904.1	45.659	4271.9
255.00	17.559	24.054	41.613	6133.7	46.189	4477.6
260.00	18.031	24.484	42.515	6366.0	46.703	4688.0
265.00	18.501	24.908	43.409	6600.7	47.202	4902.8
270.00	18.971	25.326	44.296	6838.0	47.686	5122.1
273.15	19.266	25.585	44.851	6988.6	47.984	5262.5
275.00	19.439	25.737	45.176	7077.6	48.156	5345.7
280.00	19.906	26.141	46.047	7319.5	48.612	5573.8
285.00	20.373	26.539	46.912	7563.7	49.056	5806.2
290.00	20.838	26.931	47.769	7810.0	49.487	6042.9
295.00	21.301	27.317	48.618	8058.5	49.906	6283.9
298.15	21.593	27.557	49.150	8216.1	50.165	6437.9
300.00	21.764	27.697	49.460	8309.1	50.314	6529.1

TABLE B-1[illegible]0 (CONT.)

THERMODYNAMIC FUNCTIONS FOR TRICALCIUM ALUMINATE ($3CA\ O\ .AL_2O_3$)
SOLID PHASE

GRAM MOLECULAR WT.= 270.1994 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^C)/T$ CAL / DEG MOLE	$(H_T^0-H_0^C)/T$ CAL / DEG MOLE	$(S_1-S_0^C)$ CAL / DEG MOLE	$(H_T^0-H_0^C)$ CAL / MOLE	C_P^0 CAL / DEG MOLE	$-(G_T^0-H_0^C)$ CAL / MOLE
300.00	21.764	27.697	49.460	8309.1	50.314	6529.1
310.00	22.604	28.439	51.123	8816.2	51.100	7037.0
320.00	23.598	29.159	52.757	9330.9	51.848	7551.4
330.00	24.506	29.858	54.364	9853.0	52.559	8087.1
340.00	25.408	30.535	55.943	10382.	53.235	8638.6
350.00	26.302	31.193	57.496	10918.	53.875	9205.8
360.00	27.190	31.832	59.022	11459.	54.480	9788.5
370.00	28.071	32.452	60.522	12007.	55.048	10386.
373.15	28.347	32.643	50.990	12181.	55.219	10576.
380.00	28.944	33.053	61.998	12560.	55.580	10999.
390.00	29.810	33.637	63.448	13119.	56.076	11626.
400.00	30.669	34.204	64.873	13682.	56.538	12268.
425.00	32.784	35.549	68.332	15108.	57.557	13933.
450.00	34.851	36.796	71.647	16558.	58.411	15683.
475.00	36.872	37.953	74.825	18028.	59.138	17514.
500.00	38.847	39.028	77.875	19514.	59.770	19423.
550.00	42.659	40.964	83.623	22530.	60.829	23463.
600.00	46.298	42.656	88.954	25594.	61.692	27779.
650.00	49.772	44.149	93.922	28697.	62.415	32352.
700.00	53.094	45.477	98.570	31834.	63.035	37165.
750.00	56.272	46.666	102.94	34999.	63.580	42204.
800.00	59.319	47.738	107.06	38191.	64.068	47455.
850.00	62.243	48.712	110.95	41405.	64.511	52906.
900.00	65.052	49.601	114.65	44641.	64.920	58547.
950.00	67.757	50.418	118.17	47897.	65.301	64369.
1000.00	70.362	51.171	121.53	51171.	65.659	70362.
1050.00	72.876	51.869	124.74	54462.	66.000	76519.
1100.00	75.304	52.519	127.82	57771.	66.326	82834.
1150.00	77.652	53.126	130.78	61095.	66.639	89300.
1200.00	79.925	53.695	133.62	64434.	66.942	95910.
1250.00	82.128	54.231	136.36	67789.	67.236	102660.
1300.00	84.265	54.737	139.00	71156.	67.523	109544.
1350.00	86.340	55.216	141.56	74541.	67.804	116559.
1400.00	88.356	55.670	144.03	77938.	68.079	123598.
1450.00	90.317	56.103	146.42	81349.	68.350	130960.
1500.00	92.226	56.515	148.74	84773.	68.616	138339.
1550.00	94.086	56.910	151.00	88210.	68.879	145833.
1600.00	95.899	57.288	153.19	91661.	69.139	153438.
1650.00	97.667	57.651	155.32	95124.	69.396	161151.
1700.00	99.393	58.000	157.39	98600.	69.650	168969.
1750.00	101.08	58.337	159.42	102089.	69.903	176889.
1800.00	102.73	58.661	161.39	105591.	70.153	184909.

^{C} AND S_0^C APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

King, E. G.,
Heat Capacities at Low Temperatures and Entropies at
298.16°K. of Crystalline Calcium and Magnesium Aluminates
J. Phys. Chem. 59, 218-219 (1955)

Bonnickson, K. R.,
High Temperature Heat Contents of Aluminates of Calcium and Magnesium
J. Phys. Chem. 59, 220-221 (1955)

TABLE B-121

THERMODYNAMIC FUNCTIONS FOR CALCIUM ALUMINATE ($12CA\,O \cdot 7AL_2O_3$)
SOLID PHASES

GRAM MOLECULAR WT.= 1386.6812 GRAMS CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

SOLID PHASE (ALPHA)

T DEG K	$-(G^0_T-H^C_0)/T$ CAL/DEG MOLE	$(H^0_T-H^C_0)/T$ CAL/DEG MOLE	$(S_T-S^C_0)$ CAL/DEG MOLE	$(H^0_T-H^C_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^C_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.005	0.015	0.020	0.076	0.061	0.025
10.00	0.041	0.122	0.163	1.222	0.489	0.407
15.00	0.137	0.411	0.548	6.163	1.631	2.060
20.00	0.323	0.953	1.276	19.065	3.683	6.465
25.00	0.619	1.775	2.394	44.375	6.562	15.478
30.00	1.035	2.857	3.892	85.721	10.062	31.041
35.00	1.571	4.171	5.742	145.99	14.146	54.982
40.00	2.226	5.706	7.932	228.25	18.863	89.027
45.00	2.997	7.459	10.456	335.67	24.207	134.86
50.00	3.883	9.425	13.308	471.24	30.106	194.14
55.00	4.881	11.591	16.472	637.48	36.457	268.46
60.00	5.989	13.940	19.929	836.42	43.169	359.34
65.00	7.203	16.454	23.658	1069.5	50.103	468.20
70.00	8.519	19.108	27.627	1337.6	57.112	596.32
75.00	9.931	21.875	31.806	1640.7	64.124	744.82
80.00	11.434	24.735	36.168	1978.8	71.117	914.69
85.00	13.021	27.668	40.688	2351.7	78.059	1106.8
90.00	14.687	30.658	45.345	2759.2	84.914	1321.8
95.00	16.425	33.692	50.117	3200.7	91.666	1560.4
100.00	18.231	36.757	54.988	3675.7	98.318	1823.1
105.00	20.099	39.845	59.944	4183.7	104.87	2110.4
110.00	22.025	42.948	64.972	4724.2	111.31	2422.7
115.00	24.002	46.057	70.060	5296.6	117.61	2760.3
120.00	26.028	49.167	75.196	5900.1	123.75	3123.4
125.00	28.098	52.271	80.369	6533.8	129.72	3512.3
130.00	30.209	55.361	85.570	7197.0	135.51	3927.1
135.00	32.356	58.435	90.790	7888.7	141.15	4368.0
140.00	34.536	61.487	96.023	8608.2	146.64	4835.0
145.00	36.747	64.516	101.26	9354.8	151.97	5328.2
150.00	38.984	67.518	106.50	10128.	157.16	5847.7
155.00	41.247	70.492	111.74	10926.	162.21	6393.3
160.00	43.531	73.435	116.97	11750.	167.10	6965.0
165.00	45.836	76.345	122.18	12597.	171.84	7562.9
170.00	48.158	79.222	127.38	13468.	176.44	8186.8
175.00	50.495	82.063	132.56	14361.	180.88	8836.7
180.00	52.846	84.869	137.72	15276.	185.19	9512.4
185.00	55.210	87.637	142.85	16213.	189.36	10214.
190.00	57.583	90.367	147.95	17170.	193.40	10941.
195.00	59.965	93.059	153.02	18147.	197.33	11693.
200.00	62.355	95.714	158.07	19143.	201.14	12471.
205.00	64.751	98.331	163.08	20158.	204.85	13274.
210.00	67.151	100.91	168.06	21191.	208.47	14102.
215.00	69.555	103.45	173.01	22242.	211.99	14954.
220.00	71.963	105.96	177.92	23311.	215.42	15832.
225.00	74.371	108.43	182.80	24396.	218.76	16734.
230.00	76.781	110.86	187.64	25498.	222.03	17660.
235.00	79.191	113.26	192.45	26617.	225.21	18610.
240.00	81.601	115.63	197.23	27750.	228.32	19584.
245.00	84.009	117.96	201.97	28900.	231.35	20582.
250.00	86.415	120.26	206.67	30064.	234.31	21604.
255.00	88.819	122.52	211.34	31243.	237.20	22649.
260.00	91.220	124.75	215.97	32436.	240.03	23717.
265.00	93.617	126.95	220.57	33643.	242.79	24803.
270.00	96.010	129.12	225.13	34864.	245.49	25923.
273.15	97.516	130.48	227.99	35639.	247.16	26636.
275.00	98.399	131.26	229.66	36098.	248.12	27060.
280.00	100.78	133.37	234.16	37345.	250.70	28219.
285.00	103.16	135.45	238.62	38604.	253.21	29401.
290.00	105.54	137.51	243.04	39877.	255.65	30605.
295.00	107.90	139.53	247.43	41161.	258.03	31832.
298.15	109.39	140.79	250.18	41976.	259.49	32615.
300.00	110.27	141.52	251.79	42457.	260.34	33080.

TABLE B-121 (CONT.)

THERMODYNAMIC FUNCTIONS FOR CALCIUM ALUMINATE ($12CA\ O\ .7AL_2O_3$)
SOLID PHASES

GRAM MOLECULAR WT.= 1386.6812 GRAMS CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^C_0)/T$ CAL/DEG MOLE	$(H^0_T-H^C_0)/T$ CAL/DEG MOLE	$(S_T-S^C_0)$ CAL/DEG MOLE	$(H^0_T-H^C_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^C_0)$ CAL/MOLE
SOLID PHASE (ALPHA)						
300.00	110.27	141.52	251.79	42457.	260.34	33080.
310.00	114.97	145.43	260.40	45082.	264.75	35641.
320.00	119.65	149.22	268.87	47751.	268.89	38287.
330.00	124.30	152.91	277.20	50459.	272.75	41018.
340.00	128.91	156.49	285.40	53205.	276.35	43831.
350.00	133.50	159.96	293.46	55986.	279.71	46725.
360.00	138.05	163.33	301.38	58798.	282.84	49700.
370.00	142.57	166.60	309.17	61642.	285.77	52752.
373.15	143.99	167.61	311.60	62543.	286.65	53730.
380.00	147.06	169.77	316.83	64513.	288.52	55883.
390.00	151.51	172.85	324.36	67411.	291.11	59089.
400.00	155.92	175.84	331.76	70335.	293.56	62369.
425.00	166.80	182.93	349.73	77745.	299.14	70889.
450.00	177.44	189.53	366.97	85257.	304.10	79850.
475.00	187.86	195.68	383.53	92946.	308.56	89232.
500.00	198.04	201.42	399.46	100711.	312.60	99021.
550.00	217.74	211.86	429.60	116524.	319.72	119757.
600.00	236.58	221.11	457.69	132668.	325.91	141947.
650.00	254.61	229.39	484.00	149104.	331.44	165496.
700.00	271.89	236.86	508.75	165806.	336.53	190321.
750.00	288.46	243.67	532.13	182750.	341.25	216348.
800.00	304.39	249.91	554.30	199925.	345.72	243514.
850.00	319.72	255.67	575.39	217318.	349.98	271760.
900.00	334.48	261.02	595.51	234920.	354.08	301036.
950.00	348.73	266.03	614.76	252724.	358.06	331297.
1000.00	362.50	270.72	633.22	270725.	361.93	362499.
1050.00	375.82	275.16	650.97	288916.	365.72	394607.
1100.00	388.71	279.36	668.07	307295.	369.44	427586.
1150.00	401.22	283.36	684.58	325859.	373.10	461404.
1200.00	413.35	287.17	700.53	344605.	376.72	496034.
1250.00	425.16	290.82	715.98	363530.	380.30	531449.
1300.00	436.63	294.23	730.97	382634.	383.84	567625.
1310.00	438.89	295.02	733.91	386476.	384.54	574949.
SOLID PHASE (BETA)						
1310.00	438.89	295.02	733.91	386476.	357.48	574949.
1350.00	447.79	296.93	744.72	400854.	361.41	604522.
1400.00	458.64	299.32	757.96	419047.	366.34	64209 .
1450.00	469.18	301.72	770.90	437487.	371.26	680313.
1500.00	479.45	304.12	783.57	456173.	376.18	719176.
1550.00	489.46	306.52	795.98	475105.	381.10	758665.
1600.00	499.23	308.93	808.16	494283.	386.02	798770.
1650.00	508.77	311.34	820.11	513708.	390.95	839477.
1700.00	518.10	313.75	831.86	533378.	395.87	880777.
1750.00	527.23	316.17	843.40	553294.	400.79	922660.
1800.00	536.17	318.59	854.76	573457.	405.71	965115.

H^C_0 AND S^C_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

King, E. G.,
Heat Capacities at Low Temperatures and Entropies at
298.16 °K. of Crystalline Calcium and Magnesium Aluminates
J. Phys. Chem. 59, 218-219 (1955)

Bonnickson, K. R.,
High Temperature Heat Contents of Aluminates of Calcium and Magnesium
J. Phys. Chem. 59, 220-221 (1955)

TABLE B-122

THERMODYNAMIC FUNCTIONS FOR MONOCALCIUM ALUMINATE $(CA\,O \cdot AL_2O_3)$
SOLID PHASE

GRAM MOLECULAR WT.= 158.0406 GRAMS　　CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^C_0)/T$ CAL / DEG MOLE	$(H^0_T-H^C_0)/T$ CAL / DEG MOLE	$(S_T-S^C_0)$ CAL / DEG MOLE	$(H^0_T-H^C_0)$ CAL / MOLE	C^0_P CAL / DEG MOLE	$-(G^0_T-H^C_0)$ CAL / MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.002	0.002	0.008	0.006	0.003
10.00	0.004	0.012	0.017	0.124	0.050	0.041
15.00	0.014	0.042	0.056	0.626	0.167	0.209
20.00	0.033	0.098	0.131	1.964	0.387	0.659
25.00	0.064	0.188	0.251	4.690	0.721	1.595
30.00	0.108	0.311	0.420	9.336	1.151	3.253
35.00	0.168	0.467	0.634	16.334	1.660	5.869
40.00	0.242	0.651	0.893	26.056	2.240	9.670
45.00	0.330	0.863	1.193	38.832	2.879	14.869
50.00	0.433	1.098	1.532	54.919	3.561	21.667
55.00	0.550	1.354	1.904	74.475	4.264	30.243
60.00	0.679	1.626	2.306	97.588	4.983	40.756
65.00	0.821	1.913	2.733	124.33	5.713	53.343
70.00	0.973	2.210	3.183	154.71	6.441	68.127
75.00	1.136	2.516	3.652	188.72	7.161	85.209
80.00	1.309	2.829	4.137	226.31	7.873	104.68
85.00	1.489	3.145	4.636	267.44	8.577	126.60
90.00	1.678	3.467	5.146	312.06	9.272	151.05
95.00	1.875	3.791	5.665	360.14	9.955	178.08
100.00	2.077	4.116	6.193	411.60	10.626	207.72
105.00	2.286	4.442	6.728	466.38	11.287	240.02
110.00	2.500	4.768	7.268	524.45	11.938	275.01
115.00	2.719	5.093	7.813	585.75	12.580	312.71
120.00	2.943	5.419	8.361	650.24	13.211	353.14
125.00	3.171	5.743	8.913	717.84	13.830	396.33
130.00	3.402	6.066	9.468	788.52	14.436	442.28
135.00	3.637	6.387	10.024	862.18	15.028	491.01
140.00	3.875	6.706	10.581	938.77	15.607	542.52
145.00	4.116	7.022	11.138	1018.2	16.174	596.81
150.00	4.359	7.337	11.696	1100.5	16.730	653.90
155.00	4.605	7.648	12.253	1185.5	17.274	713.77
160.00	4.853	7.958	12.810	1273.2	17.808	776.43
165.00	5.102	8.264	13.366	1363.6	18.330	841.87
170.00	5.353	8.568	13.921	1456.5	18.841	910.09
175.00	5.606	8.868	14.475	1552.0	19.341	981.08
180.00	5.860	9.166	15.026	1649.9	19.829	1054.8
185.00	6.115	9.461	15.576	1750.2	20.307	1131.3
190.00	6.372	9.752	16.124	1853.0	20.775	1210.6
195.00	6.629	10.041	16.669	1958.0	21.232	1292.6
200.00	6.886	10.326	17.213	2065.3	21.681	1377.3
205.00	7.145	10.609	17.754	2174.8	22.121	1464.7
210.00	7.404	10.888	18.292	2286.5	22.553	1554.8
215.00	7.663	11.164	18.827	2400.3	22.975	1647.6
220.00	7.923	11.437	19.360	2516.2	23.389	1743.1
225.00	8.183	11.707	19.891	2634.2	23.795	1841.2
230.00	8.443	11.974	20.418	2754.1	24.191	1942.0
235.00	8.704	12.239	20.942	2876.1	24.579	2045.4
240.00	8.964	12.500	21.464	2999.9	24.958	2151.4
245.00	[illegible]	12.758	21.982	3125.6	25.329	2260.0
250.00	9.485	13.013	22.498	3253.2	25.693	2371.2
255.00	9.745	13.265	23.010	3382.5	26.049	2485.0
260.00	10.005	13.514	23.519	3513.7	26.398	2601.3
265.00	10.265	13.760	24.025	3646.5	26.742	2720.2
270.00	10.524	14.004	24.528	3781.1	27.079	2841.6
273.15	10.688	14.156	24.844	3866.7	27.289	2919.3
275.00	10.783	14.245	25.028	3917.3	27.411	2965.5
280.00	11.042	14.483	25.525	4055.2	27.737	3091.8
285.00	11.301	14.718	26.019	4194.7	28.058	3220.7
290.00	11.559	14.951	26.510	4335.7	28.373	3352.0
295.00	11.816	15.181	26.997	4478.4	28.681	3485.8
298.15	11.978	15.325	27.303	4569.0	28.872	3571.3
300.00	12.073	15.408	27.482	4622.5	28.983	3622.0

TABLE B-122 (CONT.)

THERMODYNAMIC FUNCTIONS FOR MONOCALCIUM ALUMINATE ($CA\ O \cdot AL_2O_3$)
SOLID PHASE

GRAM MOLECULAR WT.= 158.0406 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^C_0)/T$ CAL/DEG MOLE	$(H^0_T-H^C_0)/T$ CAL/DEG MOLE	$(S_T-S^C_0)$ CAL/DEG MOLE	$(H^0_T-H^C_0)$ CAL/MOLE	C^0_p CAL/DEG MOLE	$-(G^0_T-H^C_0)$ CAL/MOLE
300.00	12.073	15.408	27.482	4622.5	28.983	3622.0
310.00	12.586	15.856	28.442	4915.2	29.566	3901.6
320.00	13.096	16.293	29.389	5213.8	30.119	4190.8
330.00	13.604	16.720	30.324	5517.6	30.638	4489.4
340.00	14.109	17.137	31.246	5826.4	31.124	4797.2
350.00	14.612	17.543	32.155	6139.9	31.576	5114.2
360.00	15.112	17.938	33.050	6457.8	31.997	5440.3
370.00	15.609	18.324	33.932	6779.8	32.388	5775.2
373.15	15.764	18.443	34.207	6882.0	32.505	5882.5
380.00	16.102	18.699	34.801	7105.5	32.752	6118.9
390.00	16.593	19.063	35.656	7434.7	33.092	6471.2
400.00	17.080	19.418	36.498	7767.3	33.410	6831.9
425.00	18.283	20.263	38.546	8611.7	34.127	7770.2
450.00	19.463	21.051	40.514	9472.8	34.751	8758.6
475.00	20.622	21.787	42.408	10349.	35.303	9795.2
500.00	21.757	22.475	44.232	11237.	35.796	10878.
550.00	23.959	23.726	47.685	13049.	36.647	13177.
600.00	26.072	24.833	50.905	14900.	37.365	15643.
650.00	28.099	25.822	53.921	16784.	37.990	18264.
700.00	30.046	26.711	56.757	18698.	38.547	21032.
750.00	31.917	27.517	59.434	20638.	39.055	23937.
800.00	33.716	28.253	61.970	22603.	39.524	26973.
850.00	35.450	28.929	64.379	24590.	39.964	30132.
900.00	37.121	29.554	66.675	26599.	40.381	33409.
950.00	38.735	30.135	68.869	28628.	40.780	36798.
1000.00	40.294	30.676	70.971	30676.	41.164	40294.
1050.00	41.804	31.185	72.988	32744.	41.536	43894.
1100.00	43.265	31.663	74.929	34830.	41.898	47592.
1150.00	44.683	32.116	76.799	36934.	42.252	51385.
1200.00	46.059	32.546	78.605	39055.	42.599	55271.
1250.00	47.396	32.955	80.351	41193.	42.940	59245.
1300.00	48.696	33.345	82.041	43349.	43.277	63305.
1350.00	49.962	33.719	83.681	45521.	43.609	67448.
1400.00	51.194	34.078	85.273	47710.	43.938	71672.
1450.00	52.396	34.424	86.820	49915.	44.263	75974.
1500.00	53.569	34.758	88.326	52136.	44.586	80353.
1550.00	54.714	35.080	89.794	54374.	44.907	84806.
1600.00	55.833	35.392	91.224	56627.	45.225	89332.
1650.00	56.926	35.695	92.621	58896.	45.542	93928.
1700.00	57.996	35.989	93.985	61181.	45.857	98594.
1750.00	59.044	36.275	95.319	63482.	46.170	103326.
1800.00	60.069	36.554	96.624	65798.	46.482	108125.

H^C_0 AND S^C_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

King, E. G.,
Heat Capacities at Low Temperatures and Entropies at
298.16°K. of Crystalline Calcium and Magnesium Aluminates
J. Phys. Chem. 59, 218-219 (1955)

Bonnickson, K. R.,
High Temperature Heat Contents of Aluminates of Calcium and Magnesium
J. Phys. Chem. 59, 220-221 (1955)

TABLE B-123

THERMODYNAMIC FUNCTIONS FOR CALCIUM DIALUMINATE $(CA\ O\ .2AL_2O_3)$
SOLID PHASE

GRAM MOLECULAR WT.= 260.0018 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^C_0)/T$ CAL/DEG MOLE	$(H^0_T-H^C_0)/T$ CAL/DEG MOLE	$(S_T-S^C_0)$ CAL/DEG MOLE	$(H^0_T-H^C_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^C_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.002	0.003	0.012	0.010	0.004
10.00	0.007	0.020	0.026	0.196	0.078	0.065
15.00	0.027	0.066	0.088	0.990	0.262	0.331
20.00	0.052	0.153	0.205	3.067	0.594	1.038
25.00	0.100	0.286	0.385	7.146	1.056	2.489
30.00	0.166	0.459	0.625	13.772	1.605	4.993
35.00	0.252	0.666	0.916	23.313	2.225	8.831
40.00	0.356	0.904	1.261	36.164	2.931	14.259
45.00	0.478	1.173	1.651	52.785	3.734	21.518
50.00	0.617	1.474	2.091	73.685	4.643	30.852
55.00	0.773	1.807	2.580	99.398	5.659	42.509
60.00	0.946	2.174	3.119	130.42	6.762	56.738
65.00	1.135	2.571	3.706	167.09	7.912	73.782
70.00	1.341	2.994	4.335	209.55	9.071	93.866
75.00	1.563	3.437	5.000	257.79	10.225	117.19
80.00	1.799	3.898	5.696	311.80	11.378	143.92
85.00	2.049	4.371	6.421	371.57	12.527	174.20
90.00	2.313	4.856	7.169	437.06	13.668	208.16
95.00	2.589	5.350	7.938	508.23	14.798	245.92
100.00	2.876	5.850	8.726	585.01	15.915	287.58
105.00	3.173	6.356	9.529	667.36	17.022	333.21
110.00	3.481	6.866	10.346	755.21	18.117	382.89
115.00	3.797	7.378	11.176	848.51	19.199	436.69
120.00	4.122	7.893	12.015	947.18	20.266	494.67
125.00	4.455	8.409	12.864	1051.1	21.315	556.86
130.00	4.795	8.925	13.720	1160.3	22.347	623.32
135.00	5.141	9.441	14.583	1274.6	23.361	694.08
140.00	5.49[illegible]	9.956	15.450	1393.9	24.356	769.16
145.00	5.852	10.470	16.322	1518.1	25.334	848.58
150.00	6.216	10.981	17.197	1647.2	26.295	932.38
155.00	6.584	11.491	18.075	1781.0	27.240	1020.6
160.00	6.957	11.997	18.954	1919.6	28.168	1113.1
165.00	7.334	12.501	19.835	2062.7	29.080	1210.1
170.00	7.715	13.002	20.717	2210.3	29.975	1311.5
175.00	8.099	13.500	21.598	2362.4	30.852	1417.3
180.00	8.486	13.993	22.479	2518.8	31.710	1527.5
185.00	8.876	14.484	23.360	2679.5	32.551	1642.1
190.00	9.269	14.970	24.239	2844.3	33.375	1761.1
195.00	9.664	15.452	25.116	3013.2	34.181	1884.5
200.00	10.061	15.930	25.992	3186.1	34.970	2012.2
205.00	10.460	16.404	26.665	3362.9	35.743	2144.4
210.00	10.861	16.874	27.735	3543.5	36.501	2280.9
215.00	11.264	17.339	28.603	3727.9	37.242	2421.7
220.00	11.668	17.800	29.467	3915.9	37.968	2566.9
225.00	12.073	18.256	30.328	4107.5	38.679	2716.4
230.00	12.479	18.707	31.186	4302.7	39.375	2870.2
235.00	12.886	19.154	32.040	4501.2	40.058	3028.2
240.00	13.294	19.597	32.891	4703.2	40.728	3190.6
245.00	13.703	20.035	33.737	4908.5	41.387	3357.1
250.00	14.112	20.468	34.580	5117.1	42.036	3527.9
255.00	14.521	20.897	35.419	5328.9	42.678	3702.9
260.00	14.931	21.322	36.254	5543.8	43.313	3882.1
265.00	15.341	21.743	37.085	5762.0	43.942	4065.5
270.00	15.752	22.160	37.912	5983.2	44.566	4252.9
273.15	16.010	22.421	38.431	6124.2	44.958	4373.2
275.00	16.162	22.573	38.735	6207.6	45.187	4444.6
280.00	16.572	22.983	39.555	6435.1	45.803	4640.3
285.00	16.983	23.388	40.371	6665.6	46.415	4840.1
290.00	17.393	23.790	41.184	6899.2	47.021	5044.0
295.00	17.803	24.189	41.993	7135.9	47.622	5251.9
298.15	18.061	24.439	42.500	7286.5	47.996	5385.0
300.00	18.213	24.585	42.798	7375.4	48.214	5469.9

TABLE B-123 (CONT.)

THERMODYNAMIC FUNCTIONS FOR CALCIUM DIALUMINATE ($CA\ O\ .2AL_2O_3$)
SOLID PHASE

GRAM MOLECULAR WT.= 260.0018 GRAMS
T DEG K = 273.15 + T DEG C
CAL=4.1840 ABS J

T DEG K	$-(G^0_T-H^C_0)/T$ CAL/DEG MOLE	$(H^0_T-H^C_0)/T$ CAL/DEG MOLE	$(S_T-S^C_0)$ CAL/DEG MOLE	$(H^0_T-H^C_0)$ CAL/MOLE	C^0_p CAL/DEG MOLE	$-(G^0_T-H^C_0)$ CAL/MOLE
300.00	18.213	24.585	42.798	7375.4	48.214	5463.9
310.00	19.032	25.366	44.398	7863.4	49.371	5899.9
320.00	19.849	26.133	45.983	8362.7	50.480	6351.8
330.00	20.665	26.887	47.553	8672.8	51.533	6819.5
340.00	21.479	27.627	49.106	9393.1	52.523	7302.8
350.00	22.290	28.352	50.642	9923.0	53.446	7801.6
360.00	23.099	29.061	52.160	10462.	54.305	8315.6
370.00	23.905	29.754	53.658	11009.	55.100	8844.7
373.15	24.158	29.969	54.127	11183.	55.339	9014.5
380.00	24.707	30.431	55.138	11564.	55.838	9388.7
390.00	25.506	31.091	56.597	12126.	56.521	9947.4
400.00	26.301	31.735	58.036	12694.	57.157	10521.
425.00	28.272	33.273	61.545	14141.	58.567	12016.
450.00	30.215	34.712	64.927	15621.	59.767	13597.
475.00	32.128	36.059	68.187	17128.	60.805	15261.
500.00	34.010	37.319	71.330	18660.	61.710	17005.
550.00	37.677	39.608	77.285	21784.	63.220	20722.
600.00	41.212	41.628	82.839	24977.	64.434	24727.
650.00	44.616	43.422	88.038	28224.	65.439	29000.
700.00	47.893	45.026	92.919	31518.	66.294	33525.
750.00	51.050	46.469	97.519	34852.	67.036	38287.
800.00	54.091	47.775	101.87	38220.	67.693	43273.
850.00	57.024	48.965	105.99	41620.	68.284	48470.
900.00	59.854	50.053	109.91	45048.	68.825	53869.
950.00	62.587	51.054	113.64	48502.	69.324	59458.
1000.00	65.230	51.980	117.21	51980.	69.790	65230.
1050.00	67.787	52.838	120.63	55480.	70.230	71176.
1100.00	70.264	53.638	123.90	59002.	70.647	77290.
1150.00	72.665	54.387	127.05	62545.	71.046	83564.
1200.00	74.994	55.089	130.08	66107.	71.430	89993.
1250.00	77.257	55.750	133.01	69687.	71.801	96571.
1300.00	79.456	56.374	135.83	73286.	72.161	103292.
1350.00	81.594	56.965	138.56	76903.	72.511	110152.
1400.00	83.676	57.527	141.20	80537.	72.854	117147.
1450.00	85.705	58.061	143.77	84188.	73.189	124272.
1500.00	87.682	58.571	146.25	87856.	73.519	131522.
1550.00	89.610	59.058	148.67	91540.	73.843	138896.
1600.00	91.493	59.525	15 .02	95240.	74.163	146388.
1650.00	93.331	59.973	153.30	98956.	74.478	153996.
1700.00	95.128	60.405	155.53	102688.	74.790	161718.
1750.00	96.885	60.820	157.71	106435.	75.099	169549.
1800.00	98.604	61.221	159.82	110198.	75.405	177487.

H^C_0 AND S^C_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

King, E. G.,
Heat Capacities at Low Temperatures and Entropies at
298.16°K. of Crystalline Calcium and Magnesium Aluminates
J. Phys. Chem. 59, 218-219 (1955)

Bonnickson, K. R.,
High Temperature Heat Contents of Aluminates of Calcium and Magnesium
J. Phys. Chem. 59, 220-221 (1955)

TABLE B-124

THFRMODYNAMIC FUNCTIONS FOR TRICALCIUM DISILICATE (3CA O .2SI O$_2$) SOLIO PHASE

GRAM MOLFCULAR WT.= 288.4078 GRAMS CAL=4.1840 ABS J

T DFG K = 273.15 + T DEG C

T OEG K	$-(G^0_T-H^C_0)/T$ CAL / OEG MOLE	$(H^0_T-H^C_0)/T$ CAL / OEG MOLE	$(S_T-S^C_0)$ CAL / OEG MOLE	$(H^0_T-H^C_0)$ CAL / MOLE	C^0_P CAL / OEG MOLE	$-(G^0_T-H^C_0)$ CAL / MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.003	0.004	0.013	0.011	0.004
10.00	0.007	0.021	0.028	0.213	0.085	0.071
15.00	0.024	0.072	0.096	1.075	0.284	0.359
20.00	0.056	0.166	0.223	3.327	0.644	1.128
25.00	0.108	0.311	0.419	7.775	1.160	2.703
30.00	0.181	0.506	0.687	15.180	1.827	5.439
35.00	0.277	0.752	1.029	26.328	2.661	9.699
40.00	0.397	1.052	1.449	42.099	3.676	15.862
45.00	0.540	1.408	1.948	63.354	4.849	24.322
50.00	0.709	1.816	2.525	90.776	6.135	35.475
55.00	0.903	2.269	3.173	124.81	7.488	49.690
60.00	1.122	2.762	3.884	165.75	8.897	67.307
65.00	1.364	3.290	4.654	213.86	10.353	88.629
70.00	1.628	3.847	5.475	269.32	11.830	113.93
75.00	1.912	4.429	6.341	332.14	13.298	143.45
80.00	2.218	5.028	7.246	402.26	14.745	177.41
85.00	2.541	5.642	8.183	479.56	16.175	215.96
90.00	2.881	6.266	9.147	563.98	17.589	259.28
95.00	3.237	6.899	10.136	655.42	18.982	307.48
100.00	3.607	7.537	11.144	753.75	20.342	360.67
105.00	3.990	8.179	12.169	858.77	21.660	418.95
110.00	4.385	8.821	13.206	970.27	22.932	482.38
115.00	4.791	9.461	14.253	1088.0	24.162	551.02
120.00	5.208	10.099	15.306	1211.8	25.336	624.91
125.00	5.633	10.732	16.365	1341.5	26.520	704.09
130.00	6.066	11.361	17.427	1477.0	27.656	788.57
135.00	6.506	11.986	18.492	1618.0	28.764	878.37
140.00	6.954	12.604	19.558	1764.6	29.840	973.49
145.00	7.407	13.217	20.623	1916.4	30.883	1073.9
150.00	7.865	13.822	21.687	2073.3	31.889	1179.7
155.00	8.328	14.421	22.749	2235.2	32.858	1290.8
160.00	8.795	15.012	23.807	2401.9	33.791	1407.2
165.00	9.266	15.594	24.860	2573.1	34.690	1528.9
170.00	9.740	16.169	25.909	2748.7	35.557	1655.8
175.00	10.217	16.735	26.952	2928.6	36.397	1787.9
180.00	10.696	17.292	27.989	3112.6	37.212	1925.3
185.00	11.177	17.842	29.019	3300.7	38.004	2067.8
190.00	11.660	18.382	30.043	3492.6	38.774	2215.5
195.00	12.145	18.915	31.060	3688.4	39.524	2368.2
200.00	12.630	19.439	32.070	3887.8	40.254	2526.1
205.00	13.117	19.956	33.072	4090.9	40.963	2688.9
210.00	13.604	20.464	34.068	4297.4	41.653	2856.8
215.00	14.091	20.965	35.056	4507.4	42.324	3029.6
220.00	14.579	21.458	36.036	4720.7	42.975	3207.3
225.00	15.066	21.943	37.009	4937.1	43.609	3389.9
230.00	15.554	22.421	37.974	5156.7	44.227	3577.4
235.00	16.041	22.891	38.932	5379.4	44.828	3769.7
240.00	16.528	23.354	39.882	5605.0	45.414	3966.7
245.00	17.014	23.810	40.824	5833.5	45.985	4168.5
250.00	17.500	24.259	41.759	6064.8	46.543	4374.9
255.00	17.985	24.701	42.686	6298.9	47.086	4586.0
260.00	18.468	25.137	43.605	6535.6	47.617	4801.8
265.00	18.951	25.566	44.517	6775.0	48.135	5022.1
270.00	19.433	25.989	45.422	7017.0	48.639	5246.9
273.15	19.736	26.252	45.988	7170.7	48.950	5390.9
275.00	19.914	26.405	46.319	7261.4	49.130	5476.3
280.00	20.393	26.815	47.208	7508.2	49.609	5710.1
285.00	20.871	27.219	48.091	7757.5	50.074	5948.4
290.00	21.348	27.617	48.965	8009.0	50.528	6191.0
295.00	21.824	28.009	49.833	8262.7	50.969	6438.0
298.15	22.123	28.256	50.379	8423.7	51.240	6595.8
300.00	22.298	28.395	50.693	8518.6	51.398	6689.3

H^C_0 ANO S^C_0 APPLY TO THE REFERENCE STATE OF THE SOLIO AT ZERO OEG K

King, E. G.,
Low Temperature Heat Capacities and Entropies at
298.15°K. of Some Crystalline Silicates Containing Calcium
J. Am. Chem. Soc. 79, 5437-5438 (1957)

TABLE B-125

THERMODYNAMIC FUNCTIONS FOR CALCIUM ORTHOSILICATE (2CA O .SI O_2)
SOLID PHASE (GAMMA)

GRAM MOLECULAR WT.= 172.2436 GRAMS CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^C_0)/T$ CAL / DEG MOLE	$(H^0_T-H^C_0)/T$ CAL / DEG MOLE	$(S_T-S^C_0)$ CAL / DEG MOLE	$(H^0_T-H^C_0)$ CAL / MOLE	C^0_P CAL / DEG MOLE	$-(G^0_T-H^C_0)$ CAL / MOLE
SOLID PHASE (GAMMA)						
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.002	0.006	0.005	0.002
10.00	0.003	0.009	0.013	0.094	0.038	0.031
15.00	0.011	0.032	0.042	0.477	0.127	0.159
20.00	0.025	0.075	0.100	1.502	0.298	0.502
25.00	0.049	0.145	0.194	3.619	0.564	1.221
30.00	0.084	0.243	0.327	7.300	0.922	2.505
35.00	0.130	0.371	0.501	12.983	1.365	4.558
40.00	0.190	0.527	0.717	21.091	1.893	7.586
45.00	0.262	0.712	0.974	32.053	2.506	11.797
50.00	0.348	0.926	1.274	46.285	3.199	17.400
55.00	0.447	1.166	1.614	64.156	3.958	24.602
60.00	0.560	1.432	1.992	85.946	4.764	33.602
65.00	0.686	1.721	2.407	111.84	5.597	44.585
70.00	0.825	2.028	2.852	141.94	6.444	57.720
75.00	0.975	2.350	3.326	176.29	7.294	73.155
80.00	1.138	2.686	3.824	214.88	8.141	91.019
85.00	1.311	3.032	4.343	257.69	8.983	111.43
90.00	1.494	3.386	4.880	304.70	9.819	134.47
95.00	1.687	3.746	5.433	355.86	10.644	160.25
100.00	1.888	4.111	5.999	411.11	11.455	188.82
105.00	2.098	4.480	6.577	470.37	12.246	220.26
110.00	2.315	4.850	7.165	533.54	13.016	254.61
115.00	2.538	5.222	7.760	600.53	13.765	291.92
120.00	2.769	5.593	8.362	671.15	14.493	332.23
125.00	3.004	5.963	8.968	745.40	15.201	375.55
130.00	3.245	6.332	9.577	823.13	15.891	421.91
135.00	3.491	6.698	10.190	904.28	16.564	471.32
140.00	3.741	7.062	10.804	988.74	17.219	523.81
145.00	3.996	7.424	11.419	1076.4	17.854	579.37
150.00	4.253	7.782	12.035	1167.3	18.470	638.00
155.00	4.514	8.136	12.650	1261.1	19.065	699.72
160.00	4.778	8.487	13.265	1357.9	19.638	764.50
165.00	5.045	8.833	13.878	1457.4	20.190	832.36
170.00	5.313	9.175	14.488	1559.7	20.723	903.28
175.00	5.584	9.512	15.096	1664.6	21.238	977.24
180.00	5.857	9.845	15.702	1772.1	21.736	1054.2
185.00	6.131	10.173	16.304	1882.0	22.220	1134.3
190.00	6.407	10.496	16.903	1994.3	22.690	1217.3
195.00	6.683	10.815	17.498	2108.9	23.147	1303.3
200.00	6.961	11.129	18.090	2225.7	23.591	1392.2
205.00	7.240	11.438	18.678	2344.8	24.024	1484.2
210.00	7.519	11.743	19.262	2465.9	24.445	1579.0
215.00	7.799	12.043	19.842	2589.2	24.854	1676.8
220.00	8.079	12.338	20.418	2714.5	25.252	1777.4
225.00	8.360	12.630	20.989	2841.7	25.639	1880.9
230.00	8.640	12.917	21.557	2970.8	26.016	1987.3
235.00	8.921	13.199	22.121	3101.8	26.383	2096.5
240.00	9.202	13.478	22.680	3234.6	26.740	2208.5
245.00	9.483	13.752	23.235	3369.2	27.090	2323.3
250.00	9.763	14.022	23.786	3505.5	27.431	2440.9
255.00	10.044	14.288	24.332	3643.5	27.763	2561.1
260.00	10.324	14.551	24.874	3783.1	28.088	2684.2
265.00	10.603	14.809	25.412	3924.4	28.405	2809.9
270.00	10.883	15.064	25.946	4067.2	28.713	2938.4
273.15	11.058	15.222	26.280	4157.9	28.902	3020.5
275.00	11.161	15.315	26.476	4211.5	29.012	3069.3
280.00	11.429	15.562	27.001	4357.3	29.302	3203.0
285.00	11.717	15.805	27.522	4504.5	29.532	3339.3
290.00	11.994	16.045	28.039	4653.1	29.852	3478.2
295.00	12.270	16.281	28.552	4803.0	30.111	3619.7
298.15	12.444	16.428	28.872	4898.1	30.270	3710.2
300.00	12.546	16.514	29.060	4954.2	30.361	3763.8

TABLE B-125 (CONT.)

THERMODYNAMIC FUNCTIONS FOR CALCIUM ORTHOSILICATE $(2CA\ O\ .SI\ O_2)$
SOLID PHASE (GAMMA)

GRAM MOLECULAR WT.= 172.2436 GRAMS CAL=4.1840 ABS J
T DEG K = 273.15 + T OEG C

T DEG K	$-(G_T^0-H_0^C)/T$ CAL/OEG MOLE	$(H_T^0-H_0^C)/T$ CAL/OEG MOLE	$(S_T-S_0^C)$ CAL/OEG MOLE	$(H_T^0-H_0^C)$ CAL/MOLE	C_P^0 CAL/OEG MOLE	$-(G_T^0-H_0^C)$ CAL/MOLE
SOLID PHASE (GAMMA)						
300.00	12.546	16.514	29.060	4954.2	30.361	3763.8
310.00	13.095	16.968	30.063	5260.2	30.832	4059.4
320.00	13.641	17.408	31.049	5570.7	31.265	4365.0
330.00	14.183	17.834	32.017	5885.4	31.667	4680.3
340.00	14.721	18.247	32.968	6203.9	32.040	5005.2
350.00	15.256	18.646	33.902	6526.1	32.389	5339.6
360.00	15.787	19.032	34.819	6851.7	32.719	5683.2
370.00	16.313	19.407	35.720	7180.4	33.031	6035.9
373.15	16.478	19.522	36.000	7284.6	33.127	6148.9
380.00	16.836	19.769	36.605	7512.2	33.329	6397.6
390.00	17.354	20.120	37.474	7847.0	33.614	6768.0
400.00	17.868	20.461	38.329	8184.5	33.888	7147.0
425.00	19.133	21.270	40.403	9039.8	34.526	8131.3
450.00	20.370	22.023	42.393	9910.4	35.112	9166.4
475.00	21.580	22.726	44.306	10795.	35.655	10250.
500.00	22.762	23.386	46.148	11693.	36.163	11381.
550.00	25.049	24.591	49.639	13525.	37.101	13777.
600.00	27.236	25.669	52.905	15402.	37.962	16341.
650.00	29.329	26.646	55.976	17320.	38.769	19064.
700.00	31.337	27.540	58.877	19278.	39.536	21936.
750.00	33.266	28.364	61.630	21273.	40.274	24949.
800.00	35.121	29.131	64.252	23305.	40.989	28097.
850.00	36.909	29.849	66.758	25372.	41.687	31373.
900.00	38.634	30.526	69.160	27473.	42.371	34771.
950.00	40.302	31.167	71.469	29609.	43.046	38287.
1000.00	41.916	31.778	73.694	31778.	43.714	41916.
1050.00	43.481	32.362	75.843	33980.	44.376	45655.
1100.00	45.000	32.923	77.923	36215.	45.030	49500.
1120.00	45.596	33.141	78.737	37118.	45.289	51068.

H_0^C ANO S_0^C APPLY TO THE REFERENCE STATE OF THE SOL10 AT ZERO OEG K

King, E. G.,
Low Temperature Heat Capacities and Entropies at
298.15°K. of Some Crystalline Silicates Containing Calcium
J. Am. Chem. Soc. 79, 5437-5438 (1957)

Kelley, K. K.,
Contributions to the Data on Theoretical Metallurgy.
XIII. High-Temperature Heat-Content, Heat-Capacity,
and Entropy Data for the Elements and Inorganic Compounds
U. S. Bur. Mines, Bull. 584, 232 pages (1960)

TABLE B-126

THERMODYNAMIC FUNCTIONS FOR CALCIUM ORTHOSILICATE (2CA O .SI O_2) SOLID PHASES

GRAM MOLECULAR WT.= 172.2436 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

SOLID PHASE (BETA)

T DEG K	$-(G_T^0-H_0^C)/T$ CAL/DEG MOLE	$(H_T^0-H_0^C)/T$ CAL/DEG MOLE	$(S_T-S_0^C)$ CAL/DEG MOLE	$(H_T^0-H_0^C)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^C)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.002	0.007	0.006	0.002
10.00	0.004	0.012	0.015	0.115	0.046	0.038
15.00	0.013	0.039	0.052	0.584	0.155	0.195
20.00	0.031	0.092	0.122	1.833	0.362	0.614
25.00	0.060	0.176	0.235	4.388	0.679	1.489
30.00	0.101	0.293	0.394	8.777	1.092	3.042
35.00	0.157	0.442	0.599	15.464	1.598	5.506
40.00	0.228	0.623	0.850	24.908	2.195	9.110
45.00	0.313	0.835	1.148	37.562	2.880	14.087
50.00	0.413	1.077	1.490	53.839	3.643	20.663
55.00	0.528	1.347	1.876	74.105	4.474	29.060
60.00	0.658	1.645	2.303	98.677	5.363	39.489
65.00	0.802	1.966	2.768	127.79	6.287	52.152
70.00	0.960	2.308	3.268	161.56	7.218	67.230
75.00	1.132	2.666	3.798	199.95	8.139	84.884
80.00	1.316	3.036	4.352	242.92	9.045	105.25
85.00	1.511	3.416	4.927	290.37	9.934	128.44
90.00	1.717	3.803	5.520	342.23	10.804	154.55
95.00	1.933	4.193	6.127	398.37	11.652	183.66
100.00	2.158	4.587	6.745	458.71	12.477	215.84
105.00	2.392	4.982	7.374	523.11	13.281	251.13
110.00	2.633	5.377	8.010	591.48	14.064	289.59
115.00	2.880	5.771	8.652	663.71	14.823	331.24
120.00	3.134	6.164	9.298	739.67	15.557	376.11
125.00	3.394	6.554	9.948	819.24	16.266	424.22
130.00	3.656	6.941	10.599	902.29	16.948	475.59
135.00	3.928	7.324	11.251	988.68	17.605	530.22
140.00	4.201	7.702	11.903	1078.3	18.237	588.10
145.00	4.478	8.076	12.553	1171.0	18.846	649.24
150.00	4.758	8.445	13.202	1266.7	19.435	713.63
155.00	5.040	8.809	13.849	1365.3	20.005	781.26
160.00	5.326	9.167	14.493	1466.7	20.556	852.12
165.00	5.613	9.520	15.134	1570.9	21.088	926.19
170.00	5.903	9.868	15.771	1677.6	21.603	1003.4
175.00	6.194	10.211	16.404	1786.9	22.099	1083.9
180.00	6.486	10.548	17.034	1898.6	22.579	1167.5
185.00	6.780	10.879	17.659	2012.6	23.042	1254.2
190.00	7.074	11.205	18.279	2129.0	23.490	1344.1
195.00	7.369	11.526	18.895	2247.5	23.924	1437.0
200.00	7.665	11.841	19.506	2368.2	24.345	1533.0
205.00	7.961	12.151	20.112	2490.9	24.755	1632.0
210.00	8.258	12.456	20.713	2615.7	25.153	1734.1
215.00	8.554	12.756	21.310	2742.4	25.542	1839.2
220.00	8.851	13.050	21.901	2871.1	25.920	1947.2
225.00	9.147	13.341	22.488	3001.6	26.290	2058.2
230.00	9.444	13.626	23.070	3134.0	26.650	2172.1
235.00	9.740	13.907	23.647	3268.1	27.002	2288.9
240.00	10.036	14.183	24.219	3404.0	27.344	2408.5
245.00	10.331	14.455	24.786	3541.5	27.678	2531.0
250.00	10.626	14.723	25.349	3680.7	28.003	2656.4
255.00	10.920	14.987	25.906	3821.6	28.320	2784.5
260.00	11.213	15.246	26.459	3963.9	28.630	2915.4
265.00	11.506	15.501	27.007	4107.8	28.932	3049.1
270.00	11.798	15.753	27.551	4253.3	29.228	3185.5
273.15	11.982	15.909	27.891	4345.6	29.411	3272.8
275.00	12.089	16.000	28.090	4400.1	29.517	3324.6
280.00	12.380	16.244	28.624	4548.4	29.801	3466.4
285.00	12.670	16.485	29.154	4698.1	30.078	3610.8
290.00	12.958	16.721	29.680	4849.2	30.350	3757.9
295.00	13.246	16.955	30.201	5001.6	30.617	3907.6
298.15	13.427	17.100	30.527	5098.3	30.782	4003.3
300.00	13.533	17.184	30.718	5155.3	30.878	4059.9

TABLE B-126 (CONT.)

THERMODYNAMIC FUNCTIONS FOR CALCIUM ORTHOSILICATE ($2CA\,O \cdot SI\,O_2$)
SOLID PHASES

GRAM MOLECULAR WT.= 172.2436 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^C)/T$ CAL/DEG MOLE	$(H_T^0-H_0^C)/T$ CAL/DEG MOLE	$(S_T-S_0^C)$ CAL/DEG MOLE	$(H_T^0-H_0^C)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_1^0-H_0^C)$ CAL/MOLE
SOLID PHASE (BETA)						
300.00	13.533	17.184	30.718	5155.3	30.878	4059.9
310.00	14.104	17.634	31.738	5466.7	31.383	4372.2
320.00	14.671	18.072	32.742	5782.9	31.865	4694.6
330.00	15.233	18.497	33.730	6103.9	32.322	5027.0
340.00	15.792	18.910	34.701	6429.3	32.753	5369.2
350.00	16.346	19.311	35.657	6758.9	33.158	5721.0
360.00	16.875	19.701	36.596	7092.4	33.540	6082.3
370.00	17.440	20.080	37.520	7429.6	33.898	6452.9
373.15	17.611	20.197	37.808	7536.5	34.006	6571.5
380.00	17.981	20.448	38.429	7770.2	34.235	6832.6
390.00	18.516	20.806	39.322	8114.3	34.553	7221.4
400.00	19.048	21.153	40.201	8461.2	34.854	7619.0
425.00	20.355	21.980	42.335	9341.4	35.544	8650.9
450.00	21.633	22.751	44.384	10238.	36.161	9735.0
475.00	22.883	23.472	46.355	11149.	36.721	10869.
500.00	24.104	24.147	48.251	12074.	37.235	12052.
550.00	26.465	25.380	51.844	13959.	38.157	14556.
600.00	28.721	26.479	55.200	15887.	38.974	17233.
650.00	30.880	27.469	58.350	17855.	39.718	20072.
700.00	32.949	28.369	61.319	19858.	40.409	23065.
750.00	34.935	29.194	64.129	21895.	41.060	26201.
800.00	36.844	29.955	66.799	23964.	41.682	29475.
850.00	38.681	30.663	69.344	26063.	42.283	32879.
900.00	40.453	31.324	71.777	28192.	42.863	36408.
950.00	42.163	31.947	74.110	30349.	43.429	40055.
970.00	42.831	32.186	75.017	31220.	43.652	41546.
SOLID PHASE (ALPHA PRIME)						
970.00	42.831	32.639	75.471	31660.	42.849	41546.
1000.00	43.830	32.951	76.781	32951.	43.180	43830.
1050.00	45.450	33.451	78.901	35123.	43.731	47723.
1100.00	47.017	33.931	80.948	37324.	44.282	51719.
1150.00	48.536	34.393	82.929	39552.	44.833	55816.
1200.00	50.009	34.839	84.848	41807.	45.384	60011.
1250.00	51.440	35.272	86.712	44090.	45.935	64300.
1300.00	52.832	35.693	88.524	46400.	46.486	68681.
1350.00	54.187	36.103	90.289	48739.	47.037	73152.
1400.00	55.507	36.503	92.010	51104.	47.588	77710.
1450.00	56.795	36.895	93.689	53497.	48.139	82352.
1500.00	58.052	37.279	95.331	55918.	48.690	87078.
1550.00	59.280	37.656	96.936	58366.	49.241	91885.
1600.00	60.482	38.026	98.508	60842.	49.792	96771.
1650.00	61.658	38.391	100.05	63346.	50.343	101735.
1700.00	62.809	38.751	101.56	65876.	50.894	106775.
1710.00	63.036	38.822	101.86	66386.	51.004	107792.
SOLID PHASE (ALPHA)						
1710.00	63.036	40.805	103.84	69776.	49.000	107792.
1750.00	63.982	40.992	104.97	71736.	49.000	111969.
1800.00	65.140	41.214	106.35	74186.	49.000	117252.
1850.00	66.272	41.425	107.70	76636.	49.000	122604.
1900.00	67.380	41.624	109.00	79086.	49.000	128021.
1950.00	68.463	41.813	110.28	81536.	49.000	133503.
2000.00	69.524	41.993	111.52	83986.	49.000	139048.

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

Todd, S. S.,
Low-temperature Heat Capacities and Entropies at
298.16°K. of Crystalline Calcium Orthosilicate, Zinc
Orthosilicate and Tricalcium Silicate
J. Am. Chem. Soc. 73, 3277-3278 (1951)

Kelley, K. K.,
Contributions to the Data on Theoretical Metallurgy.
XIII. High-Temperature Heat-Content, Heat-Capacity,
and Entropy Data for the Elements and Inorganic Compounds
U. S. Bur. Mines, Bull. 584, 232 pages (1960)

TABLE B-127

THERMODYNAMIC FUNCTIONS FOR CALCIUM FERRITE ($CA\ O \cdot FE_2O_3$)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.= 215.7716 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^C)/T$ CAL/DEG MOLE	$(H_T^0-H_0^C)/T$ CAL/DEG MOLE	$(S_T-S_0^C)$ CAL/DEG MOLE	$(H_T^0-H_0^C)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^C)$ CAL/MOLE
SOLID PHASE						
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.001	0.005	0.004	0.002
10.00	0.003	0.008	0.010	0.075	0.030	0.025
15.00	0.008	0.025	0.034	0.381	0.102	0.127
20.00	0.020	0.060	0.080	1.202	0.239	0.401
25.00	0.039	0.116	0.156	2.912	0.459	0.977
30.00	0.067	0.198	0.265	5.941	0.767	2.014
35.00	0.105	0.307	0.412	10.740	1.168	3.691
40.00	0.155	0.445	0.600	17.786	1.567	6.204
45.00	0.217	0.613	0.830	27.574	2.265	9.750
50.00	0.291	0.812	1.104	40.605	2.964	14.574
55.00	0.379	1.043	1.423	57.382	3.763	20.871
60.00	0.481	1.307	1.788	78.390	4.656	28.879
65.00	0.597	1.601	2.198	104.06	5.615	38.826
70.00	0.728	1.923	2.650	134.60	6.607	50.930
75.00	0.872	2.269	3.141	170.16	7.620	65.393
80.00	1.030	2.635	3.665	210.84	8.656	82.394
85.00	1.201	3.021	4.222	256.75	9.712	102.10
90.00	1.385	3.422	4.807	307.98	10.780	124.66
95.00	1.581	3.837	5.419	364.55	11.850	150.21
100.00	1.789	4.265	6.054	426.48	12.920	178.88
105.00	2.007	4.702	6.710	493.75	13.986	210.79
110.00	2.236	5.148	7.385	566.33	15.043	246.01
115.00	2.475	5.601	8.077	644.16	16.086	284.66
120.00	2.723	6.060	8.783	727.16	17.112	326.81
125.00	2.980	6.522	9.502	815.25	18.125	372.51
130.00	3.245	6.988	10.233	908.40	19.135	421.85
135.00	3.517	7.456	10.974	1006.6	20.152	474.86
140.00	3.797	7.928	11.725	1109.9	21.180	531.60
145.00	4.084	8.403	12.487	1218.4	22.213	592.13
150.00	4.377	8.880	13.257	1332.1	23.239	656.48
155.00	4.676	9.360	14.035	1450.8	24.239	724.71
160.00	4.980	9.840	14.820	1574.4	25.194	796.85
165.00	5.290	10.319	15.609	1702.6	26.092	872.92
170.00	5.606	10.795	16.401	1835.2	26.926	952.94
175.00	5.925	11.267	17.192	1971.8	27.696	1036.9
180.00	6.249	11.734	17.983	2112.0	28.407	1124.9
185.00	6.577	12.193	18.770	2255.7	29.067	1216.7
190.00	6.908	12.645	19.554	2402.6	29.682	1312.6
195.00	7.242	13.090	20.332	2552.5	30.260	1412.3
200.00	7.579	13.526	21.105	2705.2	30.805	1515.9
205.00	7.919	13.954	21.872	2860.5	31.318	1623.3
210.00	8.260	14.373	22.633	3018.3	31.802	1734.6
215.00	8.603	14.784	23.387	3178.5	32.255	1849.6
220.00	8.947	15.186	24.133	3340.8	32.680	1968.4
225.00	9.293	15.579	24.872	3505.2	33.076	2091.0
230.00	9.640	15.963	25.603	3671.5	33.444	2217.1
235.00	9.987	16.339	26.326	3839.6	33.786	2347.0
240.00	10.335	16.706	27.041	4009.4	34.105	2480.4
245.00	10.683	17.064	27.747	4180.6	34.402	2617.4
250.00	11.031	17.413	28.445	4353.3	34.680	2757.8
255.00	11.380	17.755	29.134	4527.4	34.941	2901.9
260.00	11.728	18.087	29.815	4702.7	35.188	3049.2
265.00	12.075	18.412	30.488	4879.3	35.421	3199.9
270.00	12.422	18.729	31.152	5056.9	35.643	3354.0
273.15	12.641	18.925	31.566	5169.4	35.777	3452.8
275.00	12.769	19.039	31.808	5235.7	35.854	3511.4
280.00	13.115	19.341	32.456	5415.4	36.055	3672.1
285.00	13.460	19.636	33.095	5596.2	36.246	3836.0
290.00	13.804	19.924	33.727	5777.9	36.429	4003.0
295.00	14.147	20.205	34.352	5960.5	36.604	4173.2
298.15	14.362	20.379	34.741	6076.0	36.711	4282.1
300.00	14.488	20.480	34.968	6143.9	36.771	4346.5

TABLE B-127 (CONT.)

THERMODYNAMIC FUNCTIONS FOR CALCIUM FERRITE (CA O $\cdot FE_2O_3$)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.= 215.7716 GRAMS   CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^C_0)/T$ CAL / DEG MOLE	$(H^0_T-H^C_0)/T$ CAL / DEG MOLE	$(S_T-S^C_0)$ CAL / DEG MOLE	$(H^0_T-H^C_0)$ CAL / MOLE	C^0_P CAL / DEG MOLE	$-(G^0_T-H^C_0)$ CAL / MOLE
			SOLID PHASE			
300.00	14.488	20.480	34.968	6143.9	36.771	4346.5
310.00	15.169	21.010	36.179	6513.2	37.084	4702.3
320.00	15.844	21.517	37.361	6885.5	37.370	5070.0
330.00	16.513	22.002	38.515	7260.5	37.632	5449.4
340.00	17.177	22.465	39.642	7638.1	37.875	5840.2
350.00	17.835	22.909	40.743	8018.0	38.100	6242.2
360.00	18.486	23.333	41.820	8400.1	38.311	6655.0
370.00	19.131	23.741	42.872	8784.2	38.508	7078.5
373.15	19.333	23.866	43.199	8905.6	38.568	7214.1
380.00	19.769	24.132	43.901	9170.2	38.694	7512.4
390.00	20.401	24.508	44.909	9558.0	38.870	7956.5
400.00	21.026	24.869	45.895	9947.5	39.036	8410.5
425.00	22.560	25.714	48.273	10928.	39.417	9587.8
450.00	24.052	26.485	50.536	11918.	39.755	10823.
475.00	25.503	27.191	52.694	12916.	40.059	12114.
500.00	26.914	27.841	54.756	13921.	40.336	13457.
550.00	29.623	29.000	58.624	15950.	40.828	16293.
600.00	32.191	30.004	62.195	18003.	41.259	19315.
650.00	34.628	30.885	65.513	20075.	41.648	22508.
700.00	36.946	31.667	68.613	22167.	42.005	25862.
750.00	39.155	32.367	71.522	24275.	42.339	29366.
800.00	41.265	33.001	74.265	26400.	42.656	33012.
850.00	43.283	33.577	76.860	28541.	42.959	36790.
900.00	45.217	34.107	79.324	30696.	43.252	40695.
950.00	47.074	34.596	81.670	32866.	43.536	44721.
1000.00	48.861	35.050	83.910	35050.	43.814	48861.
1050.00	50.581	35.474	86.055	37247.	44.086	53110.
1100.00	52.241	35.871	88.112	39458.	44.354	57465.
1150.00	53.843	36.246	90.085	41682.	44.617	61920.
1200.00	55.394	36.600	91.994	43920.	44.878	66472.
1250.00	56.895	36.936	93.831	46170.	45.136	71118.
1300.00	58.349	37.256	95.606	48433.	45.391	75854.
1350.00	59.761	37.562	97.324	50709.	45.645	80678.
1400.00	61.133	37.856	98.938	52998.	45.897	85586.
1450.00	62.466	38.137	100.60	55299.	46.148	90576.
1500.00	63.764	38.405	102.17	57613.	46.397	95645.
1510.00	64.019	38.462	102.48	58077.	46.447	96669.
			LIQUID PHASE			
1510.00	64.019	55.594	119.61	83947.	54.900	96669.
1550.00	65.472	55.576	121.05	86143.	54.900	101482.
1600.00	67.236	55.555	122.79	88888.	54.900	107578.
1650.00	68.946	55.535	124.48	91633.	54.900	113760.
1700.00	70.603	55.516	126.12	94378.	54.900	120025.
1750.00	72.212	55.499	127.71	97123.	54.900	126371.
1800.00	73.775	55.482	129.26	99868.	54.900	132796.
1850.00	75.295	55.466	130.76	102613.	54.900	139296.
1900.00	76.774	55.452	132.23	105358.	54.900	145871.
1950.00	78.215	55.437	133.65	108103.	54.900	152518.
2000.00	79.618	55.424	135.04	110848.	54.900	159236.

H^C_0 AND S^C_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

King, E. G.,
Heat Capacities at Low Temperatures and Entropies at
298.16°K. of Calcium and Magnesium Ferrites
J. Am. Chem. Soc. 76, 5849-5850 (1954)

Kelley, K. K.,
Contributions to the Data on Theoretical Metallurgy.
XIII. High-Temperature Heat-Content, Heat-Capacity,
and Entropy Data for the Elements and Inorganic Compounds
U. S. Bur. Mines, Bull. 584, 232 pages (1960)

TABLE B-128

THERMOOYNAMIC FUNCTIONS FOR DICALCIUM FERRITE (2CA O .FE_2O_3)
SOLID AND LIQUIO PHASES

GRAM MOLECULAR WT.= 271.8510 GRAMS CAL=4.1840 ABS J

T OEG K = 273.15 + T OEG C

T DEG K	$-(G^0_T-H^0_0)/T$ CAL/DEG MOLE	$(H^0_T-H^0_0)/T$ CAL/DEG MOLE	$(S_T-S^0_0)$ CAL/OEG MOLE	$(H^0_T-H^0_0)$ CAL/MOLE	C^0_P CAL/OEG MOLE	$-(G^0_T-H^0_0)$ CAL/MOLE
SOLIO PHASE						
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.001	0.003	0.004	0.014	0.011	0.004
10.00	0.007	0.022	0.029	0.218	0.087	0.072
15.00	0.024	0.073	0.097	1.095	0.289	0.366
20.00	0.057	0.169	0.226	3.381	0.652	1.148
25.00	0.110	0.315	0.425	7.867	1.164	2.746
30.00	0.184	0.508	0.691	15.227	1.798	5.508
35.00	0.279	0.744	1.023	26.054	2.553	9.767
40.00	0.396	1.024	1.420	40.956	3.426	15.850
45.00	0.535	1.344	1.878	60.462	4.390	24.072
50.00	0.695	1.699	2.394	84.961	5.422	34.730
55.00	0.875	2.088	2.962	114.81	6.533	48.098
60.00	1.074	2.507	3.581	150.44	7.728	64.435
65.00	1.292	2.957	4.249	192.19	8.978	83.991
70.00	1.529	3.432	4.961	240.24	10.245	107.00
75.00	1.782	3.929	5.711	294.64	11.514	133.66
80.00	2.052	4.442	6.494	355.38	12.782	164.16
85.00	2.337	4.970	7.307	422.45	14.045	198.65
90.00	2.636	5.509	8.145	495.80	15.293	237.27
95.00	2.949	6.056	9.005	575.35	16.524	280.14
100.00	3.274	6.610	9.884	661.02	17.739	327.36
105.00	3.610	7.169	10.778	752.72	18.937	379.01
110.00	3.956	7.731	11.687	850.36	20.115	435.16
115.00	4.312	8.294	12.606	953.83	21.271	495.89
120.00	4.677	8.858	13.535	1063.0	22.398	561.24
125.00	5.050	9.422	14.472	1177.8	23.496	631.26
130.00	5.431	9.984	15.415	1297.9	24.563	705.97
135.00	5.818	10.543	16.361	1423.3	25.600	785.41
140.00	6.211	11.099	17.310	1553.9	26.608	869.59
145.00	6.610	11.651	18.261	1689.4	27.589	958.52
150.00	7.015	12.198	19.213	1829.7	28.541	1052.2
155.00	7.423	12.740	20.164	1974.7	29.466	1150.6
160.00	7.836	13.277	21.113	2124.3	30.361	1253.8
165.00	8.253	13.808	22.061	2278.3	31.226	1361.8
170.00	8.673	14.332	23.006	2436.5	32.060	1474.4
175.00	9.096	14.851	23.947	2598.8	32.863	1591.8
180.00	9.522	15.362	24.883	2765.1	33.637	1713.9
185.00	9.949	15.866	25.815	2935.2	34.382	1840.6
190.00	10.379	16.363	26.742	3108.9	35.099	1972.0
195.00	10.811	16.852	27.662	3286.1	35.791	2108.1
200.00	11.243	17.334	28.577	3466.7	36.459	2248.7
205.00	11.677	17.808	29.485	3650.7	37.104	2393.8
210.00	12.112	18.275	30.387	3837.7	37.727	2543.5
215.00	12.547	18.734	31.282	4027.9	38.329	2697.7
220.00	12.983	19.186	32.170	4221.0	38.911	2856.3
225.00	13.419	19.631	33.050	4417.0	39.473	3019.4
230.00	13.856	20.068	33.924	4615.7	40.017	3186.8
235.00	14.292	20.498	34.790	4817.1	40.544	3358.6
240.00	14.728	20.921	35.649	5021.1	41.054	3534.7
245.00	15.164	21.337	36.501	5227.6	41.549	3715.1
250.00	15.599	21.746	37.345	5436.6	42.031	3899.7
255.00	16.033	22.149	38.182	5647.9	42.500	4088.5
260.00	16.467	22.544	39.012	5861.6	42.960	4281.5
265.00	16.900	22.934	39.834	6077.5	43.409	4478.6
270.00	17.333	23.317	40.650	6295.6	43.851	4679.8
273.15	17.605	23.556	41.160	6434.2	44.125	4808.7
275.00	17.764	23.694	41.458	6516.0	44.284	4885.1
280.00	18.194	24.066	42.260	6738.5	44.710	5094.4
285.00	18.623	24.432	43.055	6963.1	45.129	5307.7
290.00	19.052	24.792	43.844	7189.8	45.540	5524.9
295.00	19.478	25.147	44.626	7418.5	45.943	5746.1
298.15	19.747	25.368	45.115	7563.6	46.193	5887.5
300.00	19.904	25.497	45.401	7649.2	46.338	5971.2

TABLE B-128 (CONT.)

THERMODYNAMIC FUNCTIONS FOR DICALCIUM FERRITE (2CA O $\cdot FE_2O_3$)
SOLID AND LIQUID PHASES

GRAM MOLECULAR WT.= 271.8510 GRAMS
T DEG K = 273.15 + T DEG C
CAL = 4.1840 ABS J

SOLID PHASE

T DEG K	$-(G_T^0-H_0^C)/T$ CAL/DEG MOLE	$(H_T^0-H_0^C)/T$ CAL/DEG MOLE	$(S_T-S_0^C)$ CAL/DEG MOLE	$(H_T^0-H_0^C)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^C)$ CAL/MOLE
300.00	19.904	25.497	45.401	7649.2	46.338	5971.2
310.00	20.751	26.182	46.933	8116.4	47.099	6432.9
320.00	21.593	26.847	48.440	8591.0	47.818	6909.8
330.00	22.429	27.493	49.922	9072.6	48.490	7401.6
340.00	23.259	28.120	51.379	9560.6	49.114	7908.1
350.00	24.083	28.728	52.811	10055.	49.689	8429.1
360.00	24.901	29.317	54.218	10554.	50.218	8964.2
370.00	25.712	29.889	55.601	11059.	50.704	9513.4
373.15	25.966	30.065	56.031	11219.	50.849	9689.2
380.00	26.516	30.443	56.959	11568.	51.151	10076.
390.00	27.314	30.979	58.293	12082.	51.562	10652.
400.00	28.105	31.498	59.603	12599.	51.942	11242.
425.00	30.052	32.726	62.778	13909.	52.776	12772.
450.00	31.955	33.860	65.815	15237.	53.474	14380.
475.00	33.814	34.908	68.722	16581.	54.065	16062.
500.00	35.630	35.879	71.509	17940.	54.570	17815.
550.00	39.133	37.617	76.750	20689.	55.381	21523.
600.00	42.472	39.124	81.596	23474.	55.997	25483.
650.00	45.657	40.441	86.098	26287.	56.475	29677.
700.00	48.697	41.600	90.298	29120.	56.855	34088.
750.00	51.603	42.628	94.231	31971.	57.162	38702.
800.00	54.384	43.544	97.928	34836.	57.413	43507.
850.00	57.049	44.367	101.42	37712.	57.623	48492.
900.00	59.606	45.108	104.71	40597.	57.798	53645.
950.00	62.063	45.780	107.84	43491.	57.946	58960.
1000.00	64.427	46.391	110.82	46391.	58.073	64427.
1050.00	66.704	46.950	113.65	49298.	58.181	70040.
1100.00	68.901	47.463	116.36	52209.	58.275	75791.
1150.00	71.021	47.935	118.96	55125.	58.358	81674.
1200.00	73.070	48.371	121.44	58045.	58.429	87684.
1250.00	75.053	48.774	123.83	60968.	58.493	93816.
1300.00	76.973	49.149	126.12	63894.	58.549	100066.
1350.00	78.835	49.498	128.33	66823.	58.599	106427.
1400.00	80.641	49.824	130.47	69754.	58.644	112897.
1450.00	82.395	50.129	132.52	72687.	58.684	119472.
1500.00	84.099	50.415	134.51	75622.	58.721	126148.
1550.00	85.756	50.683	136.44	78559.	58.754	132922.
1600.00	87.370	50.936	138.31	81498.	58.784	139791.
1650.00	88.941	51.174	140.11	84438.	58.811	146752.
1700.00	90.472	51.399	141.87	87379.	58.836	153802.
1750.00	91.965	51.612	143.58	90321.	58.859	160938.

LIQUID PHASE

T DEG K	$-(G_T^0-H_0^C)/T$ CAL/DEG MOLE	$(H_T^0-H_0^C)/T$ CAL/DEG MOLE	$(S_T-S_0^C)$ CAL/DEG MOLE	$(H_T^0-H_0^C)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^C)$ CAL/MOLE
1750.00	91.965	72.246	164.21	126431.	74.200	160938.
1800.00	94.001	72.301	166.30	130141.	74.200	169201.
1850.00	95.982	72.352	168.33	133851.	74.200	177567.
1900.00	97.913	72.401	170.31	137561.	74.200	186034.
1950.00	99.794	72.447	172.24	141271.	74.200	194598.
2000.00	101.63	72.491	174.12	144981.	74.200	203257.

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

King, E. G.,
Heat Capacities at Low Temperatures and Entropies at
298.16°K. of Calcium and Magnesium Ferrites
J. Am. Chem. Soc. 76, 5849-5850 (1954)

Kelley, K. K.,
Contributions to the Data on Theoretical Metallurgy.
XIII. High-Temperature Heat-Content, Heat-Capacity,
and Entropy Data for the Elements and Inorganic Compounds
U. S. Bur. Mines, Bull. 584, 232 pages (1960)

TARLE B-129

THERMODYNAMIC FUNCTIONS FOR COBALT FERRITE (CO O $\cdot FE_2O_3$)
SOLIO PHASE

GRAM MOLECULAR WT.= 234.6248 GRAMS CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T	$-(G^0_T-H^C_0)/T$	$(H^0_T-H^C_0)/T$	$(S_T-S^C_0)$	$(H^0_T-H^C_0)$	C^0_P	$-(G^0_T-H^C_0)$
DEG K	CAL / DEG MOLE	CAL / 05G MOL5	CAL / DEG MOLE	CAL / MOLE	CAL / DEG MOLE	CAL / MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.002	0.006	0.005	0.002
10.00	0.003	0.010	0.013	0.098	0.039	0.033
15.00	0.011	0.033	0.044	0.496	0.132	0.166
20.00	0.026	0.078	0.104	1.557	0.308	0.522
25.00	0.051	0.150	0.200	3.740	0.581	1.266
30.00	0.086	0.251	0.337	7.522	0.945	2.592
35.00	0.134	0.381	0.515	13.327	1.390	4.706
40.00	0.195	0.539	0.734	21.553	1.914	7.812
45.00	0.269	0.724	0.993	32.592	2.515	12.115
50.00	0.356	0.937	1.293	46.825	3.191	17.814
55.00	0.457	1.175	1.631	64.611	3.935	25.108
60.00	0.570	1.438	2.008	86.271	4.739	34.190
65.00	0.696	1.724	2.420	112.08	5.590	45.245
70.00	0.835	2.032	2.867	142.23	6.473	58.449
75.00	0.986	2.358	3.344	176.82	7.367	73.964
80.00	1.149	2.699	3.848	215.90	8.263	91.932
85.00	1.323	3.052	4.376	259.45	9.158	112.48
90.00	1.508	3.416	4.925	307.48	10.055	135.72
95.00	1.703	3.790	5.492	360.01	10.957	161.76
100.00	1.907	4.171	6.077	417.06	11.863	190.68
105.00	2.120	4.558	6.678	478.64	12.769	222.56
110.00	2.341	4.952	7.293	544.74	13.671	257.48
115.00	2.570	5.351	7.920	615.33	14.564	295.51
120.00	2.806	5.753	8.559	690.36	15.447	336.70
125.00	3.049	6.158	9.207	769.78	16.319	381.11
130.00	3.298	6.566	9.864	853.53	17.180	428.79
135.00	3.554	6.975	10.528	941.56	18.028	479.77
140.00	3.815	7.384	11.199	1033.8	18.863	534.08
145.00	4.081	7.794	11.875	1130.2	19.680	591.77
150.00	4.352	8.204	12.556	1230.6	20.477	652.84
155.00	4.628	8.612	13.240	1334.9	21.253	717.33
160.00	4.908	9.019	13.927	1443.1	22.007	785.25
165.00	5.192	9.424	14.615	1554.9	22.740	856.60
170.00	5.479	9.826	15.305	1670.4	23.454	931.40
175.00	5.769	10.225	15.995	1789.4	24.149	1009.7
180.00	6.063	10.622	16.685	1911.9	24.828	1091.4
185.00	6.359	11.015	17.374	2037.7	25.491	1176.5
190.00	6.658	11.404	18.062	2166.8	26.139	1265.1
195.00	6.960	11.790	18.750	2299.1	26.771	1357.1
200.00	7.263	12.172	19.435	2434.5	27.389	1452.6
205.00	7.568	12.551	20.119	2572.9	27.990	1551.5
210.00	7.875	12.925	20.800	2714.3	28.575	1653.8
215.00	8.184	13.296	21.480	2858.6	29.142	1759.5
220.00	8.493	13.662	22.156	3005.7	29.693	1868.6
225.00	8.805	14.025	22.829	3155.5	30.227	1981.0
230.00	9.117	14.382	23.499	3308.0	30.744	2096.8
235.00	9.430	14.736	24.166	3462.9	31.244	2216.0
240.00	9.744	15.085	24.829	3620.4	31.729	2338.5
245.00	10.058	15.429	25.488	3780.2	32.198	2464.3
250.00	10.373	15.769	26.143	3942.3	32.654	2593.4
255.00	10.689	16.105	26.794	4106.7	33.098	2725.7
260.00	11.005	16.436	27.441	4273.3	33.530	2861.3
265.00	11.321	16.762	28.083	4442.0	33.951	3000.1
270.00	11.637	17.084	28.722	4612.8	34.364	3142.1
273.15	11.837	17.285	29.122	4721.4	34.619	3233.2
275.00	11.954	17.402	29.356	4785.6	34.767	3287.3
280.00	12.270	17.716	29.986	4960.5	35.163	3435.7
285.00	12.587	18.025	30.612	5137.2	35.550	3587.2
290.00	12.903	18.331	31.234	5315.9	35.929	3741.8
295.00	13.219	18.632	31.851	5496.5	36.300	3899.5
298.15	13.418	18.823	32.241	5611.2	36.529	4000.4
300.00	13.534	18.930	32.464	5678.9	36.663	4060.3

H^C_0 AND S^C_0 APPLY TO THE RFFERENCE STATE OF THE SOLID AT ZERO DEG K

King, E. G.,
Heat Capacities at Low Temperatures and Entropies of
Five Spinel Minerals
J. Phys. Chem. 60, 410-412 (1956)

TABLE B-130

THERMODYNAMIC FUNCTIONS FOR IRON COBALTITE (FE CO_2O_3)
SOLIO PHASE

GRAM MOLFCULAR WT.= 237.7110 GRAMS CAL=4.1840 ABS J

T OEG K = 273.15 + T OEG C

T DFG K	$-(G_T^0-H_0^C)/T$ CAL/OEG MOLE	$(H_T^0-H_0^C)/T$ CAL/OEG MOLE	$(S_T-S_0^C)$ CAL/OEG MOLE	$(H_T^0-H_0^C)$ CAL/MOLE	C_P^0 CAL/OEG MOLE	$-(G_T^0-H_0^C)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.002	0.007	0.005	0.002
10.00	0.003	0.010	0.014	0.105	0.042	0.035
15.00	0.012	0.035	0.047	0.530	0.141	0.177
20.00	0.028	0.083	0.111	1.668	0.330	0.558
25.00	0.054	0.160	0.214	4.001	0.619	1.355
30.00	0.092	0.267	0.359	8.002	0.993	2.771
35.00	0.143	0.401	0.544	14.033	1.429	5.013
40.00	0.207	0.560	0.766	22.382	1.919	8.274
45.00	0.283	0.740	1.023	33.307	2.459	12.734
50.00	0.371	0.941	1.312	47.053	3.048	18.559
55.00	0.471	1.161	1.632	63.870	3.687	25.908
60.00	0.582	1.400	1.983	84.022	4.382	34.933
65.00	0.704	1.658	2.363	107.79	5.131	45.784
70.00	0.837	1.934	2.771	135.39	5.916	58.607
75.00	0.981	2.226	3.207	166.97	6.716	73.543
80.00	1.134	2.532	3.666	202.55	7.518	90.715
85.00	1.297	2.849	4.146	242.15	8.321	110.24
90.00	1.469	3.175	4.644	285.77	9.130	132.20
95.00	1.650	3.510	5.160	333.46	9.947	156.71
100.00	1.838	3.853	5.691	385.25	10.771	183.83
105.00	2.035	4.202	6.236	441.18	11.599	213.64
110.00	2.238	4.557	6.795	501.25	12.428	246.21
115.00	2.449	4.917	7.366	565.46	13.255	281.61
120.00	2.666	5.282	7.947	633.79	14.079	319.89
125.00	2.889	5.650	8.539	706.24	14.899	361.10
130.00	3.118	6.021	9.139	782.78	15.715	405.29
135.00	3.352	6.395	9.747	863.38	16.525	452.50
140.00	3.591	6.771	10.363	948.00	17.324	502.77
145.00	3.835	7.149	10.984	1036.6	18.111	556.14
150.00	4.084	7.527	11.611	1129.1	18.882	612.63
155.00	4.337	7.906	12.243	1225.4	19.635	672.26
160.00	4.594	8.284	12.878	1325.4	20.369	735.06
165.00	4.855	8.661	13.516	1429.0	21.084	801.04
170.00	5.119	9.037	14.156	1536.2	21.780	870.22
175.00	5.386	9.410	14.797	1646.8	22.460	942.60
180.00	5.657	9.782	15.439	1760.8	23.123	1018.2
185.00	5.930	10.151	16.081	1878.0	23.769	1097.0
190.00	6.205	10.518	16.723	1998.5	24.400	1179.0
195.00	6.483	10.882	17.365	2122.0	25.013	1264.2
200.00	6.763	11.243	18.006	2248.6	25.610	1352.7
205.00	7.045	11.600	18.646	2378.1	26.190	1444.3
210.00	7.329	11.954	19.283	2510.4	26.752	1539.1
215.00	7.614	12.305	19.919	2645.6	27.296	1637.1
220.00	7.901	12.652	20.553	2783.4	27.823	1738.3
225.00	8.190	12.994	21.184	2923.8	28.333	1842.6
230.00	8.479	13.333	21.812	3066.7	28.826	1950.1
235.00	8.769	13.668	22.437	3212.0	29.303	2060.8
240.00	9.060	13.999	23.059	3359.7	29.765	2174.5
245.00	9.352	14.325	23.677	3509.6	30.212	2291.3
250.00	9.645	14.647	24.292	3661.8	30.646	2411.3
255.00	9.938	14.965	24.903	3816.1	31.066	2534.3
260.00	10.232	15.278	25.510	3972.4	31.474	2660.3
265.00	10.526	15.588	26.114	4130.8	31.871	2789.4
270.00	10.820	15.893	26.713	4291.1	32.256	2921.4
273.15	11.006	16.083	27.089	4393.1	32.494	3006.2
275.00	11.114	16.194	27.308	4453.3	32.632	3056.5
280.00	11.409	16.491	27.900	4617.4	32.997	3194.5
285.00	11.703	16.783	28.487	4783.3	33.352	3335.5
290.00	11.998	17.072	29.070	4950.9	33.699	3479.4
295.00	12.292	17.357	29.649	5120.2	34.036	3626.2
298.15	12.477	17.534	30.011	5227.8	34.244	3720.1
300.00	12.586	17.637	30.224	5291.2	34.364	3775.8

H_0^C AND S_0^C APPLY TO THE REFFRENCF STATE OF THF SOLIO AT ZERO OEG K

King, E. G.,
Heat Capacities at Low Temperatures and Entropies of
Five Spinel Minerals
J. Phys. Chem. 60, 410-412 (1956)

TABLE B-131

THERMODYNAMIC FUNCTIONS FOR NICKEL FERRITE ($NI\ O \cdot FE_2O_3$)
SOLID PHASE

GRAM MOLECULAR WT.= 234.4016 GRAMS CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G^0_T-H^C_0)/T$ CAL/DEG MOLE	$(H^0_T-H^C_0)/T$ CAL/DEG MOLE	$(S_T-S^C_0)$ CAL/DEG MOLE	$(H^0_T-H^C_0)$ CAL/MOLE	C^0_P CAL/DEG MOLE	$-(G^0_T-H^C_0)$ CAL/MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.001	0.001	0.005	0.004	0.002
10.00	0.003	0.008	0.011	0.085	0.034	0.028
15.00	0.010	0.029	0.038	0.431	0.115	0.143
20.00	0.023	0.068	0.091	1.365	0.272	0.454
25.00	0.044	0.132	0.176	3.305	0.518	1.408
30.00	0.076	0.223	0.299	6.690	0.848	2.281
35.00	0.119	0.340	0.459	11.901	1.247	4.160
40.00	0.173	0.482	0.655	19.270	1.711	6.930
45.00	0.239	0.647	0.886	29.110	2.236	10.769
50.00	0.317	0.835	1.152	41.738	2.826	15.849
55.00	0.406	1.045	1.451	57.475	3.480	22.343
60.00	0.507	1.278	1.785	76.656	4.202	30.418
65.00	0.619	1.532	2.151	99.602	4.984	40.245
70.00	0.743	1.808	2.551	126.56	5.805	51.98
75.00	0.877	2.102	2.980	157.68	6.641	65.802
80.00	1.023	2.412	3.435	192.98	7.480	81.828
85.00	1.179	2.735	3.914	232.47	8.320	100.19
90.00	1.344	3.069	4.413	276.19	9.167	121.00
95.00	1.520	3.412	4.932	324.16	10.022	144.35
100.00	1.703	3.764	5.468	376.42	10.882	170.35
105.00	1.896	4.124	6.019	432.98	11.742	199.06
110.00	2.096	4.489	6.585	493.83	12.597	230.56
115.00	2.304	4.860	7.164	558.94	13.445	264.93
120.00	2.519	5.236	7.754	628.27	14.286	302.22
125.00	2.740	5.614	8.354	701.79	15.120	342.49
130.00	2.968	5.996	8.963	779.46	15.946	385.78
135.00	3.201	6.380	9.581	861.23	16.762	432.14
140.00	3.440	6.765	10.205	947.06	17.566	481.60
145.00	3.684	7.151	10.835	1036.9	18.355	534.19
150.00	3.933	7.537	11.470	1130.6	19.127	589.96
155.00	4.186	7.923	12.110	1228.1	19.879	648.90
160.00	4.444	8.308	12.753	1329.3	20.612	711.06
165.00	4.706	8.692	13.398	1434.2	21.326	776.43
170.00	4.971	9.074	14.045	1542.6	22.020	845.04
175.00	5.239	9.454	14.693	1654.4	22.697	916.88
180.00	5.511	9.831	15.342	1769.5	23.356	991.97
185.00	5.785	10.205	15.990	1887.9	23.999	1070.3
190.00	6.062	10.576	16.639	[illegible]	[illegible]	1151.9
195.00	6.342	10.944	17.286	[illegible]	[illegible]	1236.7
200.00	6.624	11.309	17.933	[illegible]	[illegible]	1324.7
205.00	6.907	11.670	18.578	[illegible]	[illegible]	[illegible]
210.00	7.193	12.028	19.221	2525.9	26.973	[illegible]
215.00	7.480	12.382	19.862	2662.1	27.522	1608.2
220.00	7.769	12.732	20.501	2801.1	28.056	1709.1
225.00	8.059	13.078	21.137	2942.6	28.575	1813.2
230.00	8.350	13.421	21.771	3086.8	29.079	1920.5
235.00	9.642	13.759	22.401	3233.4	29.570	2030.9
240.00	8.935	14.094	23.029	3382.5	30.048	2144.5
245.00	9.229	14.424	23.653	3533.9	30.513	2261.2
250.00	9.524	14.750	24.274	3687.6	30.966	2381.0
255.00	9.819	15.073	24.892	3843.5	31.407	2503.9
260.00	10.115	15.391	25.506	4001.6	31.838	2629.9
265.00	10.411	15.705	26.116	4161.9	32.258	2759.0
270.00	10.708	16.015	26.723	4324.2	32.668	2891.1
273.15	10.895	16.209	27.104	4427.5	32.921	2975.9
275.00	11.004	16.322	27.326	4488.5	33.068	3026.2
280.00	11.301	16.624	27.926	4654.9	33.460	3164.4
285.00	11.598	16.923	28.521	4823.1	33.842	3305.5
290.00	11.895	17.218	29.113	4993.3	34.215	3449.6
295.00	12.192	17.509	29.701	5165.2	34.580	3596.6
298.15	12.379	17.691	30.070	5274.5	34.805	3690.7
300.00	12.489	17.797	30.285	5339.0	34.935	3746.6

H^C_0 AND S^C_0 APPLY TO THE REFERENCE STATE OF THE SOLID AT ZERO DEG K

King, E. G.,
Heat Capacities at Low Temperatures and Entropies of
Five Spinel Minerals
J. Phys. Chem. 60, 410-412 (1956)

TABLE B-132

THERMODYNAMIC FUNCTIONS FOR FERRIC OXIDE (FE_2O_3)
SOLID PHASES

GRAM MOLECULAR WT.= 159.6922 GRAMS CAL=4.1840 ABS J
T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^C)/T$ CAL DEG-MOLE	$(H_T^0-H_0^C)/T$ CAL DEG-MOLE	$(S_T-S_0^C)$ CAL DEG-MOLE	$(H_T^0-H_0^C)$ CAL MOLE	C_P^0 CAL DEG-MOLE	$-(G_T^0-H_0^C)$ CAL MOLE
			SOLID PHASE (ALPHA)			
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.000	0.000	0.000	0.001	0.001	0.000
10.00	0.001	0.002	0.003	0.022	0.012	0.006
15.00	0.003	0.010	0.013	0.157	0.043	0.042
20.00	0.007	0.024	0.031	0.471	0.091	0.149
25.00	0.015	0.047	0.062	1.168	0.199	0.374
30.00	0.027	0.086	0.113	2.585	0.380	0.800
35.00	0.044	0.145	0.189	5.073	0.628	1.544
40.00	0.068	0.225	0.293	8.995	0.952	2.737
45.00	0.101	0.326	0.427	14.692	1.335	4.526
50.00	0.141	0.449	0.590	22.428	1.767	7.055
55.00	0.190	0.589	0.780	32.422	2.238	10.468
60.00	0.248	0.748	0.996	44.871	2.748	14.896
65.00	0.315	0.922	1.237	59.961	3.293	20.470
70.00	0.390	1.112	1.502	77.851	3.867	27.309
75.00	0.474	1.316	1.789	98.666	4.461	35.529
80.00	0.565	1.531	2.096	122.48	5.068	45.235
85.00	0.665	1.757	2.422	149.36	5.683	56.524
90.00	0.772	1.992	2.764	179.32	6.301	69.484
95.00	0.886	2.235	3.122	212.36	6.916	84.193
100.00	1.007	2.485	3.492	248.47	7.530	100.72
105.00	1.135	2.740	3.874	287.66	8.144	119.13
110.00	1.268	2.999	4.267	329.92	8.760	139.43
115.00	1.407	3.263	4.670	375.26	9.374	161.82
120.00	1.552	3.530	5.082	423.65	9.984	186.20
125.00	1.701	3.801	5.502	475.08	10.586	212.65
130.00	1.856	4.073	5.929	529.50	11.179	241.27
135.00	2.014	4.347	6.362	586.86	11.763	271.95
140.00	2.178	4.622	6.800	647.11	12.337	304.85
145.00	2.345	4.898	7.243	710.21	12.901	339.96
150.00	2.515	5.174	7.689	776.11	13.456	377.28
155.00	2.689	5.450	8.139	844.75	13.999	416.85
160.00	2.867	5.725	8.592	916.07	14.529	458.68
165.00	3.047	6.000	9.047	990.02	15.045	502.78
170.00	3.230	6.274	9.504	1066.5	15.546	549.16
175.00	3.416	6.545	9.962	1145.5	16.034	597.82
180.00	3.604	6.816	10.420	1226.8	16.509	648.77
185.00	3.795	7.084	10.879	1310.5	16.972	702.02
190.00	3.987	7.350	11.337	1396.5	17.424	757.56
195.00	4.181	7.614	11.796	1484.7	17.866	815.39
200.00	4.378	7.876	12.253	1575.2	18.296	875.51
205.00	4.575	8.135	12.710	1667.7	18.716	937.92
210.00	4.774	8.392	13.166	1762.3	19.125	1002.6
215.00	4.975	8.646	13.621	1858.9	19.523	1069.6
220.00	5.176	8.898	14.074	1957.5	19.911	1138.8
225.00	5.379	9.147	14.526	2058.0	20.290	1210.3
230.00	5.583	9.393	14.976	2160.4	20.658	1284.1
235.00	5.788	9.637	15.424	2264.6	21.018	1360.1
240.00	5.993	9.877	15.870	2370.6	21.369	1438.3
245.00	6.199	10.115	16.314	2478.3	21.710	1518.8
250.00	6.406	10.351	16.756	2587.6	22.042	1601.5
255.00	6.613	10.583	17.196	2698.7	22.366	1686.3
260.00	6.821	10.813	17.633	2811.3	22.680	1773.4
265.00	7.029	11.039	18.068	2925.5	22.985	1862.7
270.00	7.237	11.263	18.501	3041.1	23.282	1954.1
273.15	7.369	11.403	18.772	3114.8	23.465	2012.8
275.00	7.446	11.485	18.931	3158.3	23.571	2047.7
280.00	7.655	11.703	19.358	3276.8	23.852	2143.4
285.00	7.864	11.918	19.782	3396.8	24.126	2241.2
290.00	8.073	12.131	20.204	3518.1	24.393	2341.2
295.00	8.282	12.341	20.624	3640.7	24.653	2443.3
298.15	8.414	12.472	20.886	3718.6	24.815	2508.7
300.00	8.491	12.549	21.040	3764.6	24.908	2547.4

TABLE B-132 (CONT.)

THERMODYNAMIC FUNCTIONS FOR FERRIC OXIDE (FE_2O_3)
SOLID PHASES

GRAM MOLECULAR WT.= 159.6922 GRAMS   CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^C)/T$ CAL/DEG MOLE	$(H_T^0-H_0^C)/T$ CAL/DEG MOLE	$(S_T-S_0^C)$ CAL/DEG MOLE	$(H_T^0-H_0^C)$ CAL/MOLE	C_P^0 CAL/DEG MOLE	$-(G_T^0-H_0^C)$ CAL/MOLE
			SOLID PHASE (ALPHA)			
300.00	8.491	12.549	21.040	3764.6	24.908	2547.4
310.00	8.910	12.955	21.865	4016.1	25.398	2762.0
320.00	9.327	13.351	22.679	4272.5	25.863	2984.7
330.00	9.744	13.737	23.481	4533.3	26.301	3215.5
340.00	10.160	14.113	24.273	4798.4	26.710	3454.3
350.00	10.574	14.478	25.052	5067.4	27.093	3700.9
360.00	10.987	14.834	25.821	5340.2	27.450	3955.3
370.00	11.398	15.179	26.577	5616.4	27.787	4217.3
373.15	11.527	15.286	26.813	5704.1	27.890	4301.4
380.00	11.807	15.515	27.323	5895.8	28.108	4486.8
390.00	12.215	15.842	28.057	6178.5	28.416	4763.7
400.00	12.620	16.160	28.780	6464.1	28.714	5047.9
425.00	13.623	16.920	30.543	7191.0	29.429	5789.6
450.00	14.610	17.634	32.244	7935.3	30.106	6574.5
475.00	15.582	18.307	33.889	8696.0	30.751	7401.3
500.00	16.537	18.945	35.482	9472.6	31.370	8268.6
550.00	18.399	20.129	38.528	11071.	32.546	10120.
600.00	20.198	21.210	41.408	12726.	33.664	12119.
650.00	21.935	22.210	44.145	14436.	34.740	14258.
700.00	23.616	23.142	46.758	16200.	35.785	16531.
750.00	25.243	24.019	49.262	18015.	36.808	18932.
800.00	26.820	24.850	51.670	19880.	37.815	21456.
850.00	28.350	25.642	53.992	21796.	38.809	24098.
900.00	29.837	26.401	56.238	23761.	39.792	26854.
950.00	31.284	27.131	58.416	25775.	40.766	29720.
			SOLID PHASE (BETA)			
950.00	31.284	27.300	58.584	25935.	36.000	29720.
1000.00	32.696	27.735	60.431	27735.	36.000	32696.
1050.00	34.059	28.129	62.187	29535.	36.000	35762.
			SOLID PHASE (GAMMA)			
1050.00	34.059	28.129	62.187	29535.	33.558	35762.
1100.00	35.373	28.377	63.751	31215.	33.646	38911.
1150.00	36.640	28.608	65.248	32900.	33.734	42136.
1200.00	37.862	28.824	66.686	34588.	33.822	45434.
1250.00	39.043	29.025	68.068	36282.	33.910	48803.
1300.00	40.185	29.215	69.400	37979.	33.998	52240.
1350.00	41.291	29.394	70.685	39682.	34.086	55743.
1400.00	42.363	29.563	71.926	41388.	34.174	59308.
1450.00	43.403	29.723	73.127	43099.	34.262	62935.
1500.00	44.413	29.876	74.290	44814.	34.350	66620.
1550.00	45.395	30.022	75.417	46534.	34.438	70363.
1600.00	46.351	30.161	76.512	48258.	34.526	74161.

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

Gronvold, F., and Westrum, Jr., E. F.,
Alpha-Ferric Oxide: Low Temperature Heat Capacity and Thermodynamic Functions
J. Am. Chem. Soc. 81, 1780-1783 (1959)

Kelley, K. K.,
Contributions to the Data on Theoretical Metallurgy.
XIII. High-Temperature Heat-Content, Heat-Capacity, and Entropy Data for the Elements and Inorganic Compounds
U. S. Bur. Mines, Bull. 584, 232 pages (1960)

TABLE B-133

THERMODYNAMIC FUNCTIONS FOR POTASSIUM CHROMATE ($K_2CR\ O_4$)
SOLID PHASE

GRAM MOLECULAR WT.= 194.1976 GRAMS　　CAL=4.1840 ABS J

T DEG K = 273.15 + T DEG C

T DEG K	$-(G_T^0-H_0^C)/T$ CAL / DEG MOLE	$(H_T^0-H_0^C)/T$ CAL / DEG MOLE	$(S_T-S_0^C)$ CAL / DEG MOLE	$(H_T^0-H_0^C)$ CAL / MOLE	C_P^0 CAL / DEG MOLE	$-(G_T^0-H_0^C)$ CAL / MOLE
0.00	0.000	0.000	0.000	0.000	0.000	0.000
5.00	0.004	0.013	0.017	0.063	0.050	0.021
10.00	0.033	0.099	0.133	0.992	0.389	0.334
15.00	0.109	0.311	0.420	4.666	1.143	1.637
20.00	0.242	0.645	0.886	12.894	2.184	4.835
25.00	0.430	1.074	1.504	26.853	3.437	10.753
30.00	0.670	1.587	2.257	47.620	4.899	20.103
35.00	0.958	2.174	3.132	76.098	6.507	33.530
40.00	1.290	2.818	4.108	112.73	8.142	51.594
45.00	1.661	3.498	5.159	157.41	9.721	74.735
50.00	2.065	4.196	6.262	209.81	11.224	103.27
55.00	2.498	4.900	7.398	269.50	12.632	137.41
60.00	2.955	5.598	8.553	335.89	13.901	177.28
65.00	3.430	6.281	9.711	408.25	15.019	222.94
70.00	3.920	6.941	10.861	485.88	16.018	274.37
75.00	4.420	7.577	11.998	568.30	16.938	331.52
80.00	4.929	8.190	13.119	655.17	17.802	394.32
85.00	5.443	8.779	14.223	746.23	18.614	462.68
90.00	5.961	9.347	15.308	841.23	19.377	536.52
95.00	6.481	9.894	16.375	939.92	20.092	615.74
100.00	7.002	10.421	17.423	1042.1	20.766	700.24
105.00	7.523	10.929	18.452	1147.5	21.407	789.94
110.00	8.043	11.419	19.462	1256.1	22.022	884.73
115.00	8.561	11.893	20.454	1367.7	22.614	984.53
120.00	9.077	12.352	21.429	1482.2	23.183	1089.2
125.00	9.590	12.796	22.386	1599.5	23.728	1198.8
130.00	10.101	13.227	23.327	1719.4	24.247	1313.1
135.00	10.608	13.644	24.252	1841.9	24.740	1432.0
140.00	11.111	14.049	25.160	1966.8	25.209	1555.6
145.00	11.611	14.441	26.052	2094.0	25.657	1683.6
150.00	12.107	14.822	26.929	2223.3	26.086	1816.1
155.00	12.599	15.192	27.792	2354.8	26.500	1952.9
160.00	13.087	15.552	28.639	2488.3	26.898	2094.0
165.00	13.571	15.902	29.473	2623.8	27.285	2239.2
170.00	14.051	16.242	30.293	2761.1	27.660	2388.7
175.00	14.527	16.574	31.100	2900.4	28.026	2542.2
180.00	14.998	16.897	31.895	3041.4	28.382	2699.6
185.00	15.465	17.212	32.677	3184.2	28.730	2861.1
190.00	15.928	17.519	33.448	3328.7	29.069	3026.4
195.00	16.387	17.820	34.207	3474.9	29.400	3195.5
200.00	16.842	18.113	34.956	3622.7	29.723	3368.5
205.00	17.293	18.400	35.693	3772.1	30.038	3545.1
210.00	17.740	18.681	36.421	3923.0	30.345	3725.4
215.00	18.183	18.956	37.139	4075.5	30.643	3909.3
220.00	18.622	19.225	37.846	4229.5	30.933	4096.7
225.00	19.057	19.488	38.545	4384.8	31.215	4287.7
230.00	19.488	19.746	39.234	4541.6	31.489	4482.2
235.00	19.915	19.999	39.914	4699.7	31.755	4680.0
240.00	20.339	20.246	40.585	4859.1	32.016	4881.3
245.00	20.759	20.489	41.248	5019.8	32.272	5085.9
250.00	21.175	20.727	41.902	5181.8	32.523	5293.8
255.00	21.588	20.961	42.549	5345.1	32.771	5504.9
260.00	21.997	21.191	43.188	5509.5	33.017	5719.2
265.00	22.403	21.416	43.819	5675.2	33.262	5936.7
270.00	22.805	21.638	44.443	5842.2	33.506	6157.4
273.15	23.057	21.775	44.832	5948.0	33.660	6298.0
275.00	23.204	21.856	45.060	6010.3	33.751	6381.2
280.00	23.600	22.070	45.670	6179.7	33.996	6608.0
285.00	23.992	22.282	46.274	6350.3	34.242	6837.9
290.00	24.382	22.490	46.872	6522.1	34.488	7070.7
295.00	24.768	22.695	47.463	6695.1	34.736	7306.6
298.15	25.010	22.823	47.833	6804.8	34.892	7456.7
300.00	25.151	22.898	48.049	6869.4	34.984	7545.4

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

Popov, M. M., and Kolesov, V. P.,
The Determination of the True Specific Heat of Solid
Materials at Low Temperatures
J. Gen. Chem. (USSR) 26, 2665-2672 (1956)

SELECTED THERMOCHEMICAL VALUES

Donald D. Wagman

In the preceding semiannual report (NBS Report 8504 dated 1 July 1964) a selection of values from the data prepared by the Chemical Thermodynamic Properties Group for the revision of NBS Circular 500, Selected Values of Chemical Thermodynamic Properties, was presented. Since that report, data on an additional number of compounds have been critically evaluated and values selected. In order to make these values available to research groups prior to completion we have presented the results on compounds of possible interest to this program in the accompanying table.

These new data will form a self-consistent set of thermodynamic tables; extreme caution should be used if they are combined with values from other sources.

"Selected Thermochemical Values"

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
			kcal/mole		cal/deg mole	
As	c,α		0	0	8.4	5.89
	β,amorp		1.0			
	γ,cubic		3.5			
	g	72.04	72.3	62.4	41.61	4.968
As^+	g	298.38	300.12			
As_2	g	53.30	53.1	41.1	57.2	8.366
As_4	g		34.4	22.1	75.	
AsO	g	16.88	16.72			
AsO_2^- std state, m = 1	aq		-102.54	-83.66	9.9	
AsO_4^{---} std state, m = 1	aq		-212.27	-155.00	-38.9	
As_2O_5	c		-221.05	-187.0	25.2	27.85
As_4O_6	c,octah		-314.04	-275.46	51.2	45.72
	c,monocl		-313.0	-275.82	56.	
	g		-289.0	-262.4	91.	
AsH_3	g	17.70	15.88	16.47	53.22	9.10
$HAsO_2$ std state, unionized, m = 1	aq		-109.1	-96.25	30.1	
$HAsO_4^{--}$ std state unionized, m = 1	aq		-216.62	-170.82	-0.4	
$H_2AsO_3^-$ std state, unionized, m = 1	aq		-170.84	-140.35	26.4	
$H_2AsO_4^-$ std state unionized, m = 1	aq		-217.39	-180.04	28.	
H_3AsO_4	c		-216.6			
AsF_3	l		-228.55	-217.29	43.31	30.25
	g	-218.68	-220.04	-216.46	69.07	15.68
$AsCl_2$	g	16.	16.			
$AsCl_3$	l		-72.9	-61.37	49.6	
	g	-61.42	-61.80	-58.77	78.17	18.10
$AsBr_3$	c		-47.2			
	g		-31.	-28.	86.94	18.92

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
			kcal/mole		cal/deg mole	
AsI_3	c	-13.91	-13.9	-14.2	50.92	25.28
As_2S_3	c		-40.4	-40.3	39.1	27.8
AsN	g	47.	46.9	40.1	53.9	7.27
$NH_4H_2AsO_4$	c		-253.3	-199.1	41.12	36.13
in 660 H_2O	aq		-249.1			
$(NH_4)_2HAsO_4$	c		-282.4			
in 660 H_2O	aq		-279.8			
$(NH_4)_3AsO_4$	c		-307.4			
Sb std state	c, III	0	0	0	10.92	6.03
	g	62.63	62.7	53.1	43.06	4.97
Sb^+	g	261.91	263.46			
Sb_2	g	56.76	53.3	44.7	60.90	8.70
Sb_4	g	50.2	49.0	33.8	84.	
SbO	g	48.	47.7			
SbO^+ std state, m = 1	aq			-42.33		
SbO_2^- std state, m = 1	aq			-81.32		
Sb_2O_4	c		-216.9	-190.2	30.4	27.39
Sb_2O_5	c		-232.3	-198.2	29.9	28.11
Sb_4O_6	c, cubic		-344.3	-303.1	52.8	
	c, orthorh		-338.7	-299.5	58.8	48.46
Sb_6O_{13}	c		-670.6			
SbH_3	g	36.62	34.68	35.31	55.61	9.81
$Sb(OH)_3$	c			-163.8		
SbF	g	-11.	-11.29			
SbF_3	c		-218.8			
in 200 H_2O	aq		-217.7			
H_3SbF_6	aq		-448.4			
SbCl	g	-6.	-6.22			
$SbCl_2$	g	-18.	-18.5			
$SbCl_3$	c		-91.34	-77.37	44.0	25.8
	g	-74.57	-75.0	-72.0	80.71	18.33

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
			kcal/mole		cal/deg mole	
$SbCl_5$	l		-105.2	-83.7	72.	
	g	-93.70	-94.25	-79.91	96.04	28.95
SbOCl	c		-89.4			
	g	-25.	-25.5			
$SbBr_3$	c		-62.0	-57.2	49.5	
	g		-46.5	-53.5	89.09	19.17
in CS_2	l		-58.4			
SbI_3	c		-24.0			
	aq		-23.6			
Sb_2S_3 black	c		-41.8	-41.5	43.5	28.65
orange	amorp		-35.2			
Sb_2Te_3	c		-13.5	-13.2	56.	
SbN	g	64.	63.66			
Bi	c	0	0	0	13.56	6.10
	g	49.56	49.5	40.2	44.669	4.968
Bi^+	g	217.6	219.1			
Bi_2	g		52.5			
Bi_2O_3	c		-137.16	-118.0	36.2	27.13
$Bi(OH)_3$	c		-170.0			
BiF	g					
BiCl	c		-31.2	-25.9	22.6	
$BiCl^{++}$ std state, m = 1	aq			-14.64		
$BiCl_2^+$ std state, m = 1	aq			-49.1		
$BiCl_3$	c		-90.6	-75.3	42.3	25.
	g	-63.32	-63.5	-61.2	85.74	19.04
in $HCl \cdot 25H_2O$	aq		-101.7			
BiOCl	c		-87.7	-77.0	28.8	
$Bi(OH)_2Cl$	c			-128.71		
$BiBr_3$	c					26.
$BiBr^{++}$ std state, m = 1	aq			-8.1		
$BiBr_2^+$ std state, m = 1	aq			-35.9		

Substance	State	ΔHf°_0	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
			kcal/mole		cal/deg mole	
$BiBr_3$ std state unionized, m = 1	aq			-63.3		
BiI	g					
BiI_3	c			-41.9		
BiS	g		43.	29.	68.	
Bi_2S_3	c		-34.2	-33.6	47.9	29.2
$Bi_2(SO_4)_3$	c		-608.1			
BiSe	g		42.0			
Bi_2Se_3	c		-2.2			
BiTe	g		42.8			
Bi_2Te_3	c		-18.5	-18.4	62.36	28.8
CH_4	g	-15.970	-17.88	-12.13	44.492	8.439
$HCOO^-$ std state, m = 1	aq		-101.71	-83.87	22.	
HCO_3^- std state, m = 1	aq		-165.39	-140.26	21.8	
HCOOH	l		-101.51	-86.38	30.82	23.67
	g		-90.48			
in 1 H_2O	aq		-101.699			
2 H_2O	aq		-101.715			
3 H_2O	aq		-101.697			
5 H_2O	aq		-101.667			
10 H_2O	aq		-101.642			
50 H_2O	aq		-101.654			
100 H_2O	aq		-101.666			
1000 H_2O	aq		-101.681			
CH_3OH	l		-57.04	-39.76	30.3	19.5
	g		-48.06			
Si	c	0	0.	0.	4.50	4.78
	g	107.86	108.9	98.3	40.12	5.318
Si^+	g	295.83	298.35			
Si_2	g	141.32	142.	128.	54.92	8.22

Substance	State	$\Delta H f_0^\circ$	$\Delta H f^\circ$	$\Delta G f^\circ$	S°	C_p°
		0°K	298.15°K			
			kcal/mole		cal/deg mole	
Si_3	g	146.4	147.			12.9
SiO	g	-24.08	-23.8	-30.2	50.55	7.15
SiO_2 α, quartz	c		-217.72	-204.75	10.00	10.62
cristobalite	c		-217.37	-204.46	10.20	10.55
trydimite	c		-217.27	-204.42	10.4	10.66
glass	amorp		-215.94	-203.33	11.2	10.6
	g		-77.			
SiH	g	86.	86.28			
SiH_4	g	10.30	8.2	13.6	48.88	10.24
Si_2H_6	g	23.04	19.2	30.4	65.14	19.31
Si_3H_8	l		22.1			
	g		28.9			
H_2SiO_3	c		-284.1	-261.1	32.	
H_4SiO_4	c		-354.0	-318.6	46.	
SiF	g	1.	1.7	-5.8	53.94	7.80
SiF_2	g	-147.75	-148.	-150.	60.38	10.49
SiF_4	g	-384.66	-385.98	-375.88	67.49	17.60
std state, m = 1	aq			-384.2		
SiF_6^{--} std state, m = 1	aq		-571.0	-525.7	29.2	
$SiHF_3$	g				64.96	14.47
SiH_3F	g				56.95	11.33
H_2SiF_6	aq		-570.			
SiCl	g	45.				
$SiCl_4$	l		-164.2	-148.16	57.3	34.73
	g	-156.51	-157.03	-147.47	79.02	21.57
SiH_3Cl	g				59.88	12.20
$SiHCl_3$	l		-128.9	-115.34	54.4	
	g	-121.40	-122.6	-115.2	74.99	18.12
$SiBr_4$	l		-109.3	-106.1	66.4	
	g		-99.3	-103.2	90.29	23.21
SiH_3Br	g				62.69	12.63

Substance	State	ΔHf°_0	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
			kcal/mole		cal/deg mole	
$SiHBr_3$	l		-85.0	-80.4	59.3	
	g		-75.9	-78.5	83.28	19.30
SiI_4	c		-45.3			
SiS	g	26.6	26.88	14.56	53.43	7.71
SiS_2	c		-49.5			
$SiSe_2$	c		-7.			
SiN	g	116.	116.68	109.41	51.78	7.21
$(NH_4)_2SiF_6$ hexagonal	c		-640.94	-565.38	66.98	54.52
cubic	c		-640.67	-565.40	67.99	59.25
in 555 H_2O	aq		-633.60			
1500 H_2O	aq		-633.20			
SiC β,cubic	c	-15.36	-15.6	-15.0	3.97	6.42
α,hexagonal	c		-15.0	-14.4	3.94	6.38
	g	175.6	177.			
$Si(CH_3)_4$	l		-63.	-24.	66.27	48.78
	g		-57.15	-23.93	85.78	34.39
$Si(C_2H_5)_4$	l		-68.			
$SiH(OCH_3)_3$	l		-199.			
$Si(OCH_3)_4$	l		-302.			
$Si(OC_2H_5)_4$	l		-334.			
$SiF_4 \cdot N(CH_3)_3$	c		-419.4			
$SiCl(CH_3)_3$	l		-91.5	-58.93	66.5	
	g		-84.32	-58.23	88.2	
Sn white	c		0	0	12.32	6.45
gray	c		-0.50	0.03	10.55	6.16
	g	72.18	72.2	63.9	40.243	5.081
Sn^+	g	241.54	243.04			
Sn^{++} in aq HCl, m = 1	aq		-2.1	-6.5	-4.	
Sn^{++++} in aq HCl, m = 1	aq		7.3	0.6	-28.	
SnO	c		-68.3	-61.4	13.5	10.59
SnO_2	c		-138.8	-124.2	12.5	12.57

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
			kcal/mole		cal/deg mole	
SnH_4	g	41.78	38.9	45.0	54.39	11.70
$Sn(OH)_2$ ppt	c		-134.1	-117.5	37.	
$Sn(OH)_4$ ppt	c		-265.3			
$SnCl_2$	c		-77.7			
in aq HCl	aq		-78.8			
$SnCl_2 \cdot 2H_2O$	c		-220.2			
$SnCl_4$	l		-122.2	-105.2	61.8	39.5
	g	-112.16	-112.7	-103.3	87.4	23.5
in aq HCl	aq		-152.5	-124.9	26.	
$SnCl_6^{--}$	aq		-231.9			
Sn(OH)Cl std state, m=1	aq		-108.4	-93.7	30.	
$SnBr_2$	c		-58.2			
in aq HBr, m = 1	aq		-58.8	-57.8	45.	
$SnBr_4$	c		-90.2	-83.7	63.2	
	g		-75.2	-79.2	98.43	24.71
Sn(OH)Br std state,m=1	aq		-97.4	-86.7	35.	
SnI_2	c		-34.3			
in aq HCl	aq		-28.5			
SnI_4	c					20.3
	g				106.6	25.2
SnS	c		-24.	-23.5	18.4	11.77
	g		28.5			
SnS_2	c				20.9	16.76
$Sn(SO_4)_2$	c		-389.4			
	aq		-354.2			
SnSe	c		-21.7			
	g		30.8			
SnTe	c		-14.6			
	g		38.4			
$(NH_4)_2SnCl_6$	c		-295.6			
	aq		-293.9			

Substance	State	ΔHf°_0	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
			kcal/mole		cal/deg mole	
$(NH_4)_2SnBr_6$	c				120.2	63.97
$SnH_2(CH_3)_2$	l		14.5			
	g		21.			
$SnH(CH_3)_3$	l		-2.1			
	g		5.			
$Sn(CH_3)_4$	l		-12.5			
	g		-4.5			
$Sn(C_2H_5)_4$	l		-22.9			
	g		-10.9			
$Sn_2(CH_3)_6$	g		-21.6			
$Sn(CH_3)_2Cl_2$	c		-80.4			
$Sn(CH_3)_3Br$	l		-45.2			
$Sn(CH_3)_3I$	l		-32.4			
in CCl_4			-31.2			
AgBr	c		-23.99	-23.16	25.6	
AgI	c		-14.78	-15.82	27.6	13.58
Na_2CO_3	c		-270.9		32.5	26.41
std state, m = 1	aq		-276.62			
in 15 H_2O			-278.80			
20 H_2O			-278.66			
50 H_2O			-277.83			
100 H_2O			-277.28			
1000 H_2O			-276.53			
$Na_2CO_3 \cdot H_2O$	c		-342.4			
$Na_2CO_3 \cdot 10H_2O$	c		-976.5			
$NaCHO_2$	c		-159.13		24.80	19.76
in 400 H_2O	aq		-158.97			
$NaCHO_2 \cdot 2H_2O$			-300.7			
Na_2SiF_6	c		-695.4	-656.7	44.7	
in 630 H_2O	aq		-685.1			

Substance	State	ΔHf_0°	ΔHf°	ΔGf°	S°	C_p°
		0°K	298.15°K			
			kcal/mole		cal/deg mole	
KH_2PO_4	c		-366.0		32.23	
K_2CO_3	c		-274.3		37.4	27.65
in 50 H_2O			-281.65			
100 H_2O			-281.58			
1000 H_2O			-281.17			
2000 H_2O			-281.0			
$K_2CO_3 \cdot \frac{1}{2}H_2O$	c		-310.7			
$KCHO_2$	c		-162.3			
	aq		-161.8			
K_2SnCl_6	c		-355.6			
	aq		-352.5			

APPENDIX IV

LIST OF IONIZATION POTENTIALS OR ELECTRON AFFINITIES OF LIGHT ELEMENT COMPOUNDS

(A Revision of Appendix IV, NBS Report 8504, dated July 1, 1964)

Charles W. Beckett and Esther C. Cassidy

Ionization potential and electron affinity data for substances formed from elements of the first and second rows of the periodic table were given in Appendix IV of the above NBS Report 8504. In Table 1 of the present list, we have revised some of the values in the light of information received subsequent to the printing of the last report. We have also added ionization potentials or electron affinities of a number of substances which were not included in the former list. We are indebted to Dr. W. C. Price [45] for many of these corrections and additional values, to Dr. L. M. Branscomb [49] for pre-publication information on the electron affinity of OH, and to Drs. J. L. Margrave and T. C. Ehlert [56] for pre-publication information on AlF_2. Other values included here were taken from the recent report entitled "A Survey of Ionization Potentials of Combustion Products" by O'Bryan and Brown [44], from a Russian volume by Vedeneev et al [50], and from a number of recent publications as indicated by references [44] through [64] of the following list of references. In some cases the bibliography has been annotated with the formula of the substances and the ionization potentials or electron affinities.

In addition to the above, recent theoretical estimates of the electron affinities for negative ions of elements in the third row of the periodic table are given in Table 2. The values presented were taken from a paper by E. Clementi [65].

As stated earlier, the data given in these tables were assembled to provide a listing of values which are useful in determining what substances are likely to be important in high-temperature research. The substances listed in this preliminary survey were limited to those expected to be present in high-temperature ionized gases containing metals in addition to stable gases. The substances expected in flames were of special interest in view of their pertinence to current practical problems in the missile and space field, as indicated by Jones et al [66] in their review of the 1962 American Rocket Society Conference on ions in flames and rocket exhausts. For more detailed and comprehensive discussion of ionization in flames and high-temperature combustion systems, the reader is referred to the AIAA Progress Series entitled Ionization in High-Temperature Gases edited by Shuler and Fenn [67], to a recent paper by Miller and Calcote on "Negative-Ion Formation in Hydrocarbon Flames" [68], and to the works of Knewstubb, Sugden and Green [69, 70, 71] on ion observations in flames and electrical discharges. Branscomb [72], Nicolet [73, 74], and Whitten and Poppoff [75] have reviewed the closely related ionization phenomena in the upper atmosphere. These phenomena also occur in combustion and exhaust processes (see Calcote [76], Sugden [77], Van Tiggelen [78], and Smith and Gatz [79]), in electrically conducting gases (see Berry [80] and Franklin [81]), and in other applications including magnetohydrodynamic devices for power generation (see Brogan [82] and Moore [83]).

A selected list of ionized (or readily ionizable) substances is given below. This summary includes some of the heavier elements having low ionization potentials. Small amounts of these elements in a mixture are likely to have large effects on electron density at 2000 to 4000°K. Ions observed in flames and the upper atmosphere also are listed for the convenience of the reader.

A. Elements Likely to Ionize Appreciably at 3000°K:

Cs, Rb, K, Na, Li	(3.9 to 5.4 e.v.)
Ba, Sr, Ca	(5.2 to 6.1 e.v.)
Pr, Nd, Ce, Sm, La, Eu	(5.4 to 5.7 e.v.)
In, Ga, Al, U, Tl	(5.8 to 6.1 e.v.)
V, Cr, Ti	(6.7 to 6.8 e.v.)
Zr, Hf, Th	(6.8 to 7.0 e.v.)

B. Selected Listing of Observed Negative Ions:

H^-, C^-, O^-, F^-, S^-, Cl^-, Br^-, I^-, C_2^-, C_3^-, O_2^-, NO_2^-, CN^-, OH^-, CH^-, NH^-, NH_2^-

C. Ions Observed in Hydrocarbon-Oxygen (or Air) Flames:

H_3O^+, CHO^+, $C_3H_3^+$, $C_2H_2^+$, CH_3O^+, $C_2H_7O^+$, $CH_3O_2^+$, $CH_5O_2^+$, $C_2H_3O^+$, $C_2H_3O_2^+$, $C_2H_5O_2^+$, CN^+, O^-, OH^-, C^-, C_2^-, C_3^-, CN^-, Cl^-

D. Some Ions Observed in Upper Atmosphere (at about 100 km Altitude)

O^-, O_2^-, O_3^-, NO_2^-, NO^+, N^+, N_2^+, O^+, O_2^+, H^-, OH^-

Many of the values listed in the tables probably have errors that are considerably larger than the crude estimates given in the third column. Some of these difficulties can be resolved by a more comprehensive review of the existing data. A new program on the collection and evaluation of ionization process data has been initiated at the National Bureau of Standards by Dr. Henry Rosenstock. This program will provide more comprehensive reviews of ionization potentials, electron affinities and related data.

From this preliminary survey and other surveys of ionization potential data, it appears that reliable values are available for many of the stable molecules likely to occur in combustion mixtures. Furthermore, since the ionization potentials of these stable molecules are in general greater than 10 electron volts, even errors as large as one electron volt would not significantly affect the electron and ion concentrations in equilibrium thermodynamic mixtures at combustion temperatures. More serious problems occur in the data on less stable species, such as the free radicals which may have much lower ionization potentials. There is a need for continuing search for information on substances with low ionization potentials. This will require the extension of the tables into the lower part of the periodic table. Negative ions obviously are of great importance in combustion systems as well as in many other applications involving ionized gases, yet the number of species for which we have reliable data is extremely small. Clearly much more work is needed in this area.

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* All values are given in electron volts.

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TABLE 1. PRELIMINARY LIST OF IONIZATION POTENTIALS OR ELECTRON AFFINITIES OF LIGHT ELEMENT COMPOUNDS

Formula	I.P. (or E.A.) e.v.	Est. Error e.v.		
H^-	0.754	0.001		
H	13.598			
H_2	15.426			
H_3	9.0	1.0		
O^-	1.465	0.005		
O	13.618			
O_2^-	0.46	0.1		
O_2	12.075	0.01		
O_3^-	2.89	0.2		
O_3	>11.7	1.0		
O_4	11.65	0.1	$O_4^+ = O_2 + O_2^+$	0.42 e.v.
OH^-	1.8	0.1		
OH	13.36	0.2		
H_2O^-	0.9	0.4		
H_2O	12.61	0.02		
HO_2^-	3.04	0.5		
HO_2	11.53	0.02		
H_2O_2	10.92	0.05		
OH_3	6.2	0.4		
F^-	3.448	0.005		
F	17.422			
F_2	15.7	0.2		

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.
HF	15.77	0.2
OF	13.	0.5
OF_2	13.7	0.2
OF_3	14.3	0.5
Cl^-	3.613	0.005
Cl	12.97	0.05
Cl_2	11.48	0.05
HCl	12.74	0.01
ClF_3	13.0	0.4
ClO^-	2.91	0.4
ClO	$\leq$ 10.4	0.2
ClO_2^-	3.43	0.4
ClO_2	11.1	0.4
ClO_3^-	3.96	0.4
ClO_3	11.7	0.4
ClO_4^-	5.82	0.4
ClO_3F	13.6	0.2
S^-	2.07	0.07
S	10.360	
S_2	8.3	1.
S_8	8.9	1.
SH^-	2.6	0.5

Formula	I.P. (or E.A.) e.v.	Est. Error e.v.		
HS	11.1	0.2		
H_2S	10.47	0.1		
SO^-	$\geq$ 1.1	0.1		
SO	12.1	0.3		
SO_2	12.34	0.2		
SF_6	16.15	0.5		
CS_2	10.1	0.1		
N^-	0.04	0.04		
N	14.53	0.05		
N^+	29.59	0.05		
N_2	15.580	0.005		
N_3^-	3.13	0.3		
N_4	15.07	0.1	$N_4^+ = N_2 + N_2^+$	0.5 e.v.
NH	13.10	0.1		
NH_2^-	1.22	0.5		
NH_2	11.6	0.4		
NH_3	10.154	0.05		
NH_4	4.9	0.2		
N_2H_3	7.88	0.2		
N_3H	10.3	0.2		
NO^-	0			
NO	9.267	0.01		
NO^+	30.6	0.3		

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.
NO_2^-	4.0	0.5
NO_2	10.97	0.03
N_2O	12.94	0.05
NF	12.2	0.3
NF_2	11.6	0.5
NF_3	13.0	0.3
NF_4	8.8	0.4
N_2F_4	12.0	0.3
NHF_2	12.0	0.3
P^-	0.77	0.2
P	10.486	
P_2^-	0.3	0.3
P_2	11.8	0.5
P_4	9.0	0.5
PH_3	9.98	0.05
PCl_3	12.2	0.2
PH	10.5	0.5
PF_3	9.71	0.05
PCl_3	9.91	0.05
C^-	1.25	0.03
C_2^-	3.1	1.
C_3^-	1.8	1.
C_4^-	4.0	1.

Formula	I.P. (or E.A.) e.v.	Est. Error e.v.
C	11.26	0.05
C_2	12.0	0.4
C_3	12.6	0.4
C_4	12.6	0.4
C_5	12.5	0.4
CH^-	1.65	0.4
CH	10.64	0.01
CH_2	10.396	0.01
CH_3^-	1.08	0.4
CH_3	9.84	0.01
CH_4	13.0	0.1
C_2H	11.3	0.4
C_2H_2	11.406	0.01
C_2H_3	9.45	0.05
C_2H_4	10.51	0.01
C_2H_5	8.80	0.05
C_2H_6	11.65	0.1
C_6H_6	9.247	0.05
$(C_6H_5)_2$	8.3	0.1
Pyrene	7.55	0.1
Coronene	7.6	0.1
CH_3^-	1.1	0.2
$C_6H_6^-$	0.54	0.2
$(C_6H_5)_2^-$	0.41	0.2

Formula	I.P. (or E.A.) e.v.	Est. Error e.v.
$C_{10}H_8^-$	0.65	0.2
CO	14.01	0.01
CO_2^-	3.8	0.4
CO_2	13.79	0.02
CHO	9.85	0.1
CH_2O	10.88	0.04
CH_2O_2	11.33	0.04
CH_4O	10.85	0.04
CHF_2	9.45	0.4
$CHCl_2$	9.54	0.1
CH_2F	9.37	0.3
CH_2Cl	9.70	0.09
CH_3	9.85	0.2
CH_3Cl	11.3	0.1
CF	8.91	0.2
CF_2	11.7	0.5
CF_3	10.10	0.05
CF_4	17.81	0.04
C_2F_4	10.12	0.2
C_6F_6	10.0	0.2
CCl_2F_2	11.7	0.5
CCl	9.5	0.5
CCl_2	11.0	0.5

Formula	I.P. (or E.A.) e.v.	Est. Error e.v.	
CCl_3	8.78	0.05	
CCl_4	11.47	0.1	
$COCl_2$	11.78	0.04	
CS	11.8	0.3	
CS_2	10.07	0.02	
COS	11.3	0.07	
CN^-	3.21	0.3	
CN	14.2	0.3	
HCN	13.73	0.1	
$CNCl$	12.49	0.1	
CH_3N_3	9.5	0.2	methyl azide
CH_3ON	10.84	0.1	formamide
CH_3ON	8.2	0.3	methylnitrosyl
CH_3O_2N	11.03	0.04	
CH_5N	8.97	0.04	methyl amine
C_2N	12.8	0.3	
C_3N	14.3	0.3	
C_4N	12.3	0.3	
C_5N	12.0	0.3	
C_6N	12.2	0.3	
C_3HN	11.6	0.3	cynoacetylene
CH_4S	9.44	0.1	

Formula	I.P. (or E.A.) e.v.	Est. Error e.v.
Si^-	1.4	0.2
Si	8.151	
Si_2	7.3	0.3
SiH	8.5	0.5
SiH_4	12.2	0.3
SiO	10.51	0.1
SiO_2	11.7	0.5
Si_2O_2	10.	1.0
SiF	7.26	0.1
SiF_2	11.0	0.5
SiF_3	10.6	0.5
SiF_4	15.4	0.4
Si_2F_4		
$SiCl$	< 7.0	1.0
$SiCl_2^-$	> 2.6	0.5
$SiCl_2$	10.0	0.4
$SiCl_3$	10.0	0.4
$SiCl_4$	12.0	0.4
SiC^-	4.0	1.0
SiC	9.0	0.3
SiC_2	10.2	0.3
Si_2C	9.1	0.3

Formula	I.P. (or E.A.) e.v.	Est. Error e.v.
B^-	0.3	0.1
B	8.298	
B_2	12.4	0.3
BH	9.73	0.01
BH_2	8.12	0.3
BH_3	11.3	0.4
BO	12.8	1.0
B_2O_2	13.3	0.4
B_2O_3	13.2	0.4
HBO_2	12.6	0.4
BF	11.2	0.5
BF_2	9.4	0.4
BF_3	15.6	0.4
BF_3^-	2.17	0.4
BCl	10.44	0.4
BCl_2	7.20	0.5
BCl_3	11.5	0.5
BOF	13.4	0.5
$(BOF)_3$	14.2	0.5
BN		
B_2H	10.62	0.5
B_2H_6	12,0	0.3
BOCl		

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.
BC	10.5	0.3
BC_2	10.7	0.3
B_2C	10.7	0.3
BSi	7.8	0.3
BCSi	9.9	0.3
Al^-	0.52	0.05
Al	5.986	
AlH	8.4	0.5
AlO	9.5	0.5
Al_2O	7.7	0.4
Al_2O_2	9.9	0.4
AlO_2H		
AlOF		
AlF	9.5	0.5
AlF_2	9.0	1.0
AlF_3	1[illegible].4	0.5
AlCl	9.0	1.0
$AlCl_2$	8.0	1.0
$AlCl_3$	12.0	0.8
$AlBr_3$	12.2	0.8

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.	
Be^-	(≤0.1)	0.1	Estimate
Be	9.322		
BeH	8.6	0.4	
BeH_2	11.9	0.5	
BeOH			
BeO	10.4	0.5	
Be_2O	10.5	0.5	
Be_3O_2	12.5	1.0	
$(BeO)_2$	11.1	0.4	
$(BeO)_3$	10.7	0.4	
$(BeO)_4$	11.0	0.5	
$(BeO)_5$	11.0	1.0	
$(BeO)_6$	11.0	1.0	
BeF	9.1	0.5	
BeF_2	14.7	0.4	
BeCl	9.0	1.0	
$BeCl_2$	11.0	1.0	
Be_2Cl_4	12.8	0.5	
Mg^-	(≤0.1)	0.1	Estimate
Mg	7.646		
MgH	6.83	0.08	
MgO	8.6	0.5	
MgF	7.8	0.3	

Formula	I.P.(or E.A.) e.v.	Est. Error e.v.
MgF_2	13.5	0.4
MgCl	7.0	1.0
$MgCl_2$	11.1	0.2
Li^-	0.7	0.2
Li	5.392	
Li_2	4.96	0.2
LiH	7.85	0.2
LiO	9.0	0.4
Li_2O	6.8	0.4
LiI	8.55	0.4
LiF	11.1	0.5
Na^-	0.6	0.2
Na	5.139	
Na_2	4.87	0.2
NaH	6.5	1.
NaO	7.6	1.
NaOH	9.0	1.
NaI	8.8	0.4
NaN_3	11.7	0.4
SrF	5.2	0.3
BaF	4.9	0.3

THE ELECTRON AFFINITIES FOR NEGATIVE IONS OF THE SERIES FROM POTASSIUM TO COPPER

The electron affinities for negative ions of the elements of the iron series, as taken from recent work [a] by Clementi, are given in Table 2. The affinities stated were estimated from the correlation energy of the corresponding neutral atoms and from calculations of the relativistic and the Hartree-Fock energies. The uncertainty in the data are estimated by the author to be from 0.1 to 0.35 e.v.

TABLE 2. ELECTRON AFFINITY FOR III ROW ELEMENTS

Formula	E. A. e. v.	Est. Error e. v.
$K^-(^2S)$	0.902	± 0.05
$Sc^-(^3F)$	0 [b]	
$Ti^-(^4F)$	0.391	± 0.2
$V^-(^5D)$	0.937	± 0.25
$Cr^-(^6S)$	0.980	± 0.35
$Mn^-(^5D)$	0 [b]	
$Fe^-(^4F)$	0.582	± 0.20
$Co^-(^3F)$	0.936	± 0.15
$Ni^-(^2D)$	1.276	± 0.20
$Cu^-(^1S)$	1.801	± 0.10
	1.799	± 0.08

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[a] E. Clementi, Phys. Rev. 135, A980 (1964).

[b] Clementi reported negative values, −0.142 ± 0.1 and −1.073 ± 0.20 respectively, for the affinities of $Sc^-(^3F)$ and $Mn^-(^5D)$. The value zero was assigned in this table since the negative values are probably incorrect.

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