

South Dakota School of Mines and Technology  
Department of Materials and Metallurgical Engineering

Met 320

HQ 2

Nov 1, 2007

**CLOSED BOOK and NOTES - NO CALCULATORS - SHOW ALL WORK ON THE PROBLEM SHEETS - DISCARD ALL OTHER WORK SHEETS. If there seems to be an error in the problem statement, suggest a correction and proceed with your assumed correction. Each problem is worth 20 points.**

- 1 a) Write the Fundamental equations for a *closed system* for dH

$$dU = TdS - PdV$$

$$H \equiv U + PV$$

$$dH = dU + PdV + VdP = TdS - PdV + PdV + VdP$$

$$dH = TdS + VdP$$

- b) The Definition of Chemical potential  $\mu_i \equiv \left. \frac{\partial G}{\partial n_i} \right)_{T, P, n_{other}}$

- c) The Criterion of Equilibrium at  $dT = dP = 0$

$$dG \leq 0$$

- d) What is the *Maxwell Relation* from  $dU = TdS - PdV$ ?

$$\left. \frac{\partial T}{\partial V} \right)_S = - \left. \frac{\partial P}{\partial S} \right)_V$$

- e) What are the two *Other Thermodynamic Relationship* arising from  $dU = TdS - PdV$ ?

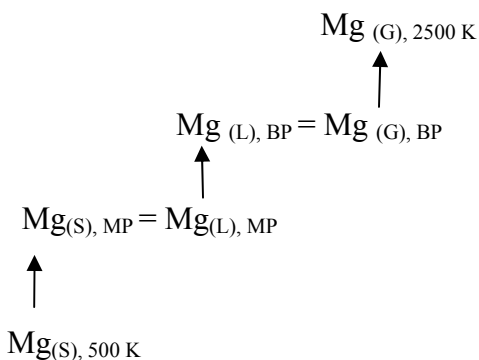
$$T = \left. \frac{\partial U}{\partial S} \right)_V \quad -P = \left. \frac{\partial U}{\partial V} \right)_S$$

2. Use the Attached JANAF tables to answer the following questions

- a)  $\Delta H^\circ$  for the reaction below at 1300 K.

$$\begin{aligned} \text{Mg}_{(s)} + \text{Cl}_{2(g)} &= \text{MgCl}_{2(l)} \\ \Delta H_{R,1300K}^\circ &= \Delta H_{\text{Form\_MgCl}_{2(l)},1300K}^\circ - \Delta H_{\text{Form\_Mg}_{(s)},1300K}^\circ - \Delta H_{\text{Form\_Cl}_{2(g)},1300K}^\circ \\ &= -141.340 - (-1.993) - (0) = -139.347 \text{ Kcal / gmole} \end{aligned}$$

- b) the amount of heat it would take to raise one gram mole of pure solid Mg at 500 K to gaseous Mg at 2500 K.



Use REFERENCE State

$$\begin{aligned} H_{2500} - H_{500} &= (H_{2500} - H_{298}) - (H_{500} - H_{298}) \\ &= 46.227 - (1.267) = 44.960 \text{ Kcal / gmole} \end{aligned}$$

- c) How much heat is required to vaporize solid Mg at 500 K to gaseous Mg at 500 K?

$$\begin{aligned} \text{Mg}_{(s), 500\text{K}} &= \text{Mg}_{(g), 500\text{K}} \\ \Delta H_{R,500\text{K}}^{\circ} &= \Delta H_{\text{Form\_Mg}_{(g)},500\text{K}}^{\circ} - \Delta H_{\text{Form\_Mg}_{(s)},500\text{K}}^{\circ} \\ &= 35.107 - (0) = 35.107 \text{ Kcal / gmole} \end{aligned}$$

3. Using only the data provided below, find the Heat of Reaction for the combustion of C<sub>2</sub>H<sub>2</sub> with oxygen C<sub>2</sub>H<sub>2</sub> (g) + 2.5O<sub>2</sub>(g) = 2CO<sub>2</sub> (g) + H<sub>2</sub>O(g) at 500 K (Draw A Calculation Schematic)

Species	Heats of Formation (Cal/g mole at 298°K)	C <sub>p</sub> (cal/ gmole °K)
C <sub>2</sub> H <sub>2</sub> (g)	+ 54,190	19.0
H <sub>2</sub> O(g)	- 57,800	10.5
CO <sub>2</sub> (g)	- 94,000	13.6
O <sub>2</sub> (g)		8.6

$$\Delta H_{R,500}^{\circ} = \Delta H_{R,298}^{\circ} + \int_{298\text{K}}^{500\text{K}} \Delta C_p dT$$

$$\Delta C_p = 2C_{p\text{CO}_2} + C_{p\text{H}_2\text{O}} - C_{p\text{C}_2\text{H}_2} - 2.5C_{p\text{O}_2}$$

$$= 2*13.6 + 10.5 - 19.0 - 2.5*8.6 = -2.80 \frac{\text{cal}}{\text{K} * \text{gmole}}$$

$$\begin{aligned} \Delta H_{R,298}^{\circ} &= 2\Delta H_{\text{Form\_CO}_2,298\text{K}}^{\circ} + \Delta H_{\text{Form\_H}_2\text{O},298\text{K}}^{\circ} - \Delta H_{\text{Form\_C}_2\text{H}_2,298\text{K}}^{\circ} - 2.5\Delta H_{\text{Form\_O}_2,298\text{K}}^{\circ} \\ &= 2*(-94,000) + (-57,800) - (54,190) - 2.5*(0) = -299,990 \text{ cal / gmole} \end{aligned}$$

$$\Delta H_{R,500}^{\circ} = -299,990 - 2.80*(500 - 298) = -300,556 \text{ cal / gmole}$$

4. The volume change for one mole of Pb going from solid to liquid is 1.25 cm<sup>3</sup>/gmole while the heat of fusion is 4,810 Joules/gmole. What would the melting temperature be at 1000 atm? The melting point is 600 K at 1 atm.



$$\frac{dP}{d \ln T} = \frac{\Delta H_{\text{Fusion}}^{\circ}}{\Delta V_{\text{Fusion}}^{\circ}}$$

$$P_2 - P_1 = \frac{\Delta H_{\text{Fusion}}^{\circ}}{\Delta V_{\text{Fusion}}^{\circ}} \ln \frac{T_2}{T_1}$$

$$\ln \frac{T_2}{T_1} = (P_2 - P_1) \frac{\Delta V_{\text{Fusion}}^{\circ}}{\Delta H_{\text{Fusion}}^{\circ}} = (1000 - 1) \text{ atm} \left[ \frac{1.25 \frac{\text{cm}^3}{\text{gmole}}}{4,810 \frac{\text{J}}{\text{gmole}}} \right] \left( \frac{8.31 \text{ J}}{82.05 \text{ cm}^3 \text{ atm}} \right)$$

$$\ln \frac{T_2}{T_1} = 0.026$$

$$\frac{T_2}{T_1} \approx 1 + 0.026 \quad (\text{Or more precisely, } 1.0263341)$$

$$T_2 = T_1 + 0.026 * T_1 = 600 + 600 * 0.026 = 600\text{K} + 15.8\text{K} = 615.8\text{K}$$

5. (Work either a or b. If both are worked only a will be graded.)

- a) The vapor pressure of ice at its melting point (273 K) is 4.579 Torr and increases to 760 Torr at its boiling point of 373 K. Determine the heat of vaporization from these data.

$$\frac{\partial \ln P}{\partial \left(\frac{1}{T}\right)} = -\frac{\Delta H_{Subl}^{\circ}}{R}$$

$$\ln \left[ \frac{P_2}{P_1} \right] = -\frac{\Delta H_{Subl}^{\circ}}{R} \left[ \frac{1}{T_2} - \frac{1}{T_1} \right]$$

$$\Delta H_{Subl}^{\circ} = -R \frac{\ln \left[ \frac{P_2}{P_1} \right]}{\left[ \frac{1}{T_2} - \frac{1}{T_1} \right]} = -8.31 \frac{J}{K * gmole} \frac{\ln \left[ \frac{760}{4.579} \right]}{\left[ \frac{1}{373K} - \frac{1}{273K} \right]} = 43,256 \frac{J}{gmole}$$

- b) The vapor pressure of silver in atm is given by the expression

$$\ln P_{Zn} = -\frac{15,205}{T} - 1.255 \ln T + 21.79 \quad Zn_{(Liq)} \rightarrow Zn_{(Gas)}$$

- i) What is the T-dependant expression for the Heat of Vaporization?

$$\frac{\partial \ln P}{\partial \left(\frac{1}{T}\right)} = -\frac{\Delta H_{vap}^{\circ}}{R} = \frac{\partial \left( \ln P_{Zn} = -\frac{15,205}{T} - 1.255 \ln T + 21.79 \right)}{\partial \left(\frac{1}{T}\right)}$$

$$\Delta H_{vap}^{\circ} = -R \frac{\partial \left( -\frac{15,205}{T} - 1.255 \ln T + 21.79 \right)}{\partial \left(\frac{1}{T}\right)}$$

$$\Delta H_{vap}^{\circ} = -R \frac{\partial \left( -\frac{15,205}{T} - 1.255 \ln T + 21.79 \right)}{\partial \left(\frac{1}{T}\right)} = -R \left[ \frac{\partial \left( -\frac{15,205}{T} \right)}{\partial \left(\frac{1}{T}\right)} + \frac{\partial (-1.255 \ln T)}{\partial \left(\frac{1}{T}\right)} \right]$$

$$\Delta H_{vap}^{\circ} = -R \left[ -15,205 - 1.255 \frac{\partial (\ln T)}{\partial \left(\frac{1}{T}\right)} \right] = -R \left[ -15,205 - 1.255 \frac{\frac{\partial T}{T}}{-\frac{\partial T}{T^2}} \right]$$

$$\Delta H_{vap}^{\circ} = (15,205 - 1.255T) R$$

- ii) What is the difference in zinc's  $C_{p(Gas)}$  and  $C_{p(Liq)}$ ?

$$\Delta C_{p_{vap}} = \frac{\partial \Delta H_{vap}^{\circ}}{\partial T} = -1.255R$$

Chlorine, Diatomic (Cl<sub>2</sub>)

(Reference State - Ideal Gas) Mol. Wt. = 70.906

T, °K.	cal. mole <sup>-1</sup> deg. <sup>-1</sup>			kcal. mole <sup>-1</sup>			Log K <sub>p</sub>
	C <sub>p</sub>	S°	-(F°-H° <sub>298</sub> )/T	H°-H° <sub>298</sub>	ΔH <sub>f</sub> °	ΔF <sub>f</sub> °	
0	.000	.000	INFINITE	- 2.194	.000	.000	.000
100	7.001	45.150	60.130	- 1.498	.000	.000	.000
200	7.576	50.156	54.016	- .772	.000	.000	.000
298	8.111	53.289	53.289	.000	.000	.000	.000
300	8.119	53.339	53.289	.015	.000	.000	.000
400	8.437	55.724	53.612	.845	.000	.000	.000
500	8.624	57.628	54.231	1.698	.000	.000	.000
600	8.741	59.212	54.933	2.567	.000	.000	.000
700	8.821	60.505	55.643	3.445	.000	.000	.000
800	8.878	61.747	56.334	4.331	.000	.000	.000
900	8.922	62.796	56.995	5.221	.000	.000	.000
1000	8.956	63.737	57.623	6.115	.000	.000	.000
1100	8.985	64.592	58.218	7.012	.000	.000	.000
1200	9.010	65.375	58.782	7.912	.000	.000	.000
1300	9.032	66.097	59.318	8.814	.000	.000	.000
1400	9.051	66.767	59.826	9.718	.000	.000	.000
1500	9.069	67.392	60.310	10.624	.000	.000	.000
1600	9.086	67.978	60.771	11.532	.000	.000	.000
1700	9.102	68.530	61.211	12.441	.000	.000	.000
1800	9.117	69.050	61.633	13.352	.000	.000	.000
1900	9.133	69.544	62.036	14.264	.000	.000	.000
2000	9.149	70.013	62.423	15.179	.000	.000	.000
2100	9.166	70.459	62.795	16.094	.000	.000	.000
2200	9.184	70.886	63.154	17.012	.000	.000	.000
2300	9.203	71.295	63.499	17.931	.000	.000	.000
2400	9.223	71.687	63.832	18.852	.000	.000	.000
2500	9.245	72.064	64.154	19.776	.000	.000	.000
2600	9.268	72.427	64.465	20.701	.000	.000	.000
2700	9.293	72.777	64.766	21.629	.000	.000	.000
2800	9.319	73.116	65.058	22.560	.000	.000	.000
2900	9.346	73.443	65.342	23.493	.000	.000	.000
3000	9.374	73.760	65.617	24.429	.000	.000	.000
3100	9.403	74.068	65.885	25.368	.000	.000	.000
3200	9.432	74.367	66.145	26.310	.000	.000	.000
3300	9.461	74.658	66.399	27.255	.000	.000	.000
3400	9.490	74.941	66.648	28.202	.000	.000	.000
3500	9.518	75.216	66.887	29.153	.000	.000	.000
3600	9.546	75.485	67.122	30.106	.000	.000	.000
3700	9.573	75.747	67.352	31.062	.000	.000	.000
3800	9.598	76.002	67.576	32.020	.000	.000	.000
3900	9.622	76.252	67.795	32.981	.000	.000	.000
4000	9.645	76.496	68.010	33.945	.000	.000	.000
4100	9.666	76.734	68.220	34.910	.000	.000	.000
4200	9.685	76.967	68.425	35.878	.000	.000	.000
4300	9.702	77.195	68.626	36.847	.000	.000	.000
4400	9.718	77.419	68.824	37.818	.000	.000	.000
4500	9.732	77.637	69.017	38.791	.000	.000	.000
4600	9.743	77.851	69.207	39.764	.000	.000	.000
4700	9.754	78.061	69.393	40.739	.000	.000	.000
4800	9.762	78.266	69.576	41.715	.000	.000	.000
4900	9.768	78.468	69.755	42.692	.000	.000	.000
5000	9.774	78.665	69.931	43.669	.000	.000	.000
5100	9.778	78.859	70.105	44.646	.000	.000	.000
5200	9.783	79.049	70.275	45.624	.000	.000	.000
5300	9.787	79.235	70.442	46.603	.000	.000	.000
5400	9.790	79.418	70.607	47.582	.000	.000	.000
5500	9.792	79.598	70.768	48.561	.000	.000	.000
5600	9.794	79.774	70.928	49.540	.000	.000	.000
5700	9.795	79.947	71.084	50.520	.000	.000	.000
5800	9.797	80.118	71.239	51.499	.000	.000	.000
5900	9.797	80.285	71.391	52.478	.000	.000	.000
6000	9.798	80.450	71.540	53.459	.000	.000	.000

CHLORINE, DIATOMIC (Cl<sub>2</sub>)

(IDEAL GAS - REFERENCE STATE)

MOL. WT. = 70.906

Ground State Configuration  $1^1\Sigma^+$   $\Delta H_{f,0}^\circ = 0$   
 $S_{298.15}^\circ = 53.29 \pm 0.01$  cal. deg.<sup>-1</sup> mole<sup>-1</sup>  $\Delta H_{f,298}^\circ = 0$

## Electronic Levels and Multiplicities

State	E cm. <sup>-1</sup>	g <sub>1</sub>
$1^1\Sigma^+$	0	1
$3^1\Pi_0^+$	18,147 ± 500	1
$3^1\Pi_1$	17,841 ± 500	2
$3^1\Pi_2$	17,560 ± 500	2

$\omega_e = 561.1$  cm.<sup>-1</sup>

$\omega_e x_e = 4.0$  cm.<sup>-1</sup>

$\sigma = 2$

$B_e = 0.2408$  cm.<sup>-1</sup>

$\alpha_e = 0.0017$  cm.<sup>-1</sup>

$r_e = 1.986$  Å

## Heat of Formation.

The heat of formation ( $\Delta H_f^\circ$ ) for Cl<sub>2</sub>(g) is zero at all temperatures, by definition.

## Heat Capacity and Entropy.

The functions adopted here were calculated by R. L. Fottler, J. Chem. Phys. 31, 1100 (1959) using a direct summation over the energy levels not including those of non-bonding states. The functions are for the naturally occurring isotopic composition.The absorption spectrum of chlorine has been observed by A. Elliott, Proc. Roy. Soc. A 127, 638 (1930); C. P. Goodeve and B. A. Stephens, Trans. Faraday Soc. 52, 1517 (1956); H. Stammreich, R. Forneris and Y. Tavares, Spectrochim. Acta, 17, 775 (1961); Y. V. Rao and P. Venkateswarlu, J. Mol. Spectr. 9, 173 (1962); and A. E. Douglas, C. K. Moller and E. P. Stoltcheff, Can. J. Phys. 41, 1174 (1963). There is disagreement over the vibrational assignments. The listed ground state spectroscopic constants for the naturally occurring isotopic composition are based upon the abundances given by D. Strominger, J. M. Hollander and G. T. Seaborg, Rev. Mod. Phys. 30, 585 (1958).The molecular structure of gaseous chlorine was determined by the sector-microphotometer method of electron diffraction by S. Shibata, J. Phys. Chem. 67, 2256 (1963). The value of  $r_e$ (Cl-Cl) was found to be 1.986 Å. The other  $r_e$  values, 1.985 - 1.989 Å, were reported by G. Herzberg, "Spectra of Diatomic Molecules", D. Van Nostrand Co., Inc., 1950; W. G. Richards and R. F. Barrow, Proc. Chem. Soc., 297 (1962), and L. S. Bartell and K. Kuchitsu, presented at the International Conference on Magnetism and Crystallography, 1961, quoted by S. Shibata, loc. cit.

Magnesium Dichloride (MgCl<sub>2</sub>)  
(Crystal) Mol. wt. = 95.218

Cl<sub>2</sub>Mg

MAGNESIUM DICHLORIDE (MgCl<sub>2</sub>)

(CRYSTAL)

MOL. WT. = 95.218

T, °K.	cal. mole <sup>-1</sup> deg. <sup>-1</sup>			kcal. mole <sup>-1</sup>			Log K <sub>p</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup>	-(F <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T	H <sup>o</sup> -H <sub>298</sub> <sup>o</sup>	ΔH <sub>f</sub> <sup>o</sup>	ΔF <sub>f</sub> <sup>o</sup>	
0	.000	.000	INFINITE	-3.288	-153.248	-153.248	INFINITE
100	9.630	6.204	35.079	-2.888	-153.703	-149.577	326.884
200	15.195	14.977	22.926	-1.590	-153.688	-145.545	159.037
298	17.060	21.422	21.422	.000	-153.350	-141.519	103.731
300	17.088	21.527	21.422	.032	-153.344	-141.446	103.038
400	18.095	26.596	22.106	1.796	-153.024	-137.528	75.138
500	18.677	30.701	23.428	3.636	-152.679	-133.692	58.434
600	19.090	34.144	24.934	5.525	-152.328	-129.928	47.324
700	19.420	37.111	26.467	7.451	-151.973	-126.222	39.406
800	19.730	39.725	27.964	9.409	-151.626	-122.569	33.483
900	20.040	42.067	29.403	11.397	-151.289	-118.956	28.889
1000	20.350	44.194	30.777	13.417	-150.982	-115.290	25.176
1100	20.654	46.148	32.087	15.467	-150.731	-111.430	22.138
1200	20.951	47.958	33.335	17.547	-150.528	-107.692	19.612
1300	21.242	49.646	34.526	19.657	-150.373	-103.982	17.480
1400	21.526	51.231	35.663	21.795	-150.263	-100.820	15.582
1500	21.805	52.726	36.751	23.962	-150.209	-98.975	13.691
1600	22.076	54.142	37.794	26.156	-150.200	-98.182	12.045
1700	22.342	55.488	38.796	28.377	-150.245	-98.435	10.597
1800	22.601	56.772	39.759	30.624	-150.345	-98.741	9.317
1900	22.854	58.001	40.687	32.997	-150.501	-99.102	8.177
2000	23.100	59.180	41.582	35.495	-150.715	-99.519	7.156

Dec. 31, 1960; Dec. 31, 1965

$\Delta H_f^o = -153.25 \pm 0.11 \text{ kcal. mole}^{-1}$   
 $S_{298.15}^o = 21.422 \text{ cal. deg.}^{-1} \text{ mole}^{-1}$   
 $T_m = 987^\circ\text{K.}$   
 $\Delta H_f^o 298.15 = -153.35 \pm 0.11 \text{ kcal. mole}^{-1}$   
 $\Delta H_m = 10.30 \pm 0.05 \text{ kcal. mole}^{-1}$   
 $\Delta H_s^o 298.15 = 57.5 \pm 1.5 \text{ kcal. mole}^{-1}$

**Heat of Formation.**  
 The adopted  $\Delta H_f^o 298.15 = -153.35 \pm 0.11 \text{ kcal. mole}^{-1}$  is from heat of solution measurements reported by C. H. Shomate and E. H. Huffman, J. Am. Chem. Soc. 65, 1625 (1943). Shomate and Huffmans heat of solution of Mg in 1 M HCl ( $\Delta H = -111.322 \pm 0.041 \text{ kcal. mole}^{-1}$ ) has been substantiated for calibration purposes by S. R. Gunn and B. B. Cunningham, J. Am. Chem. Soc., 79, 1583 (1957) ( $\Delta H = -111.3 \text{ kcal. mole}^{-1}$ ) and by E. P. Westrum Jr. and L. Eyring, J. Am. Chem. Soc., 74, 2045 (1952) ( $\Delta H = -111.27 \text{ kcal. mole}^{-1}$ ). Auxiliary heat of dilution and heat of formation data for HCl were taken from V. B. Parker, "Thermal Properties of Aqueous Uni-univalent Electrolytes", NSRDS-NBS 2, Nat'l. Bur. Stds., April 1965 and from D. D. Wagman et al., N.B.S. Technical Note 270-1, Oct. 1965.

**Heat Capacity and Entropy.**  
 High temperature heat content data by G. E. Moore, J. Am. Chem. Soc. 65, 1700 (1943) were joined by Shomate correlation with low temperature heat capacity data reported by K. K. Kelley and G. E. Moore, J. Am. Chem. Soc. 65, 1264 (1943).  $C_p(c)$  above  $T_m$  is a linear extrapolation from 700°K.  $S_{298.15}^o$  is derived from the low temperature data and is based on  $S_{53.6}^o = 2.006 \text{ cal. deg.}^{-1} \text{ mole}^{-1}$ .

**Melting Data.**  
 $\Delta H_m = 10.30 \pm 0.05 \text{ kcal. mole}^{-1}$  is taken from heat content measurements of Moore loc. cit.  $T_m = 987^\circ\text{K.}$  is from National Bureau of Standards Circular 500, 1952.

**Sublimation Data.**  
 The value of  $\Delta H_s^o 298.15$  was derived by 2nd and 3rd law analyses of vapor pressure data. See the MgCl<sub>2</sub>(g) table for details.

Cl<sub>2</sub>Mg

Magnesium Dichloride (MgCl<sub>2</sub>)

(Liquid) Mol. Wt. = 95.218

Cl<sub>2</sub>Mg

T, °K.	cal. mole <sup>-1</sup> deg. <sup>-1</sup>			kcal. mole <sup>-1</sup>			Log K <sub>p</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup>	-(F <sup>o</sup> -H <sub>298</sub> <sup>o</sup> )/T	H <sup>o</sup> -H <sub>298</sub> <sup>o</sup>	ΔH <sub>f</sub> <sup>o</sup>	ΔF <sub>f</sub> <sup>o</sup>	
0							
100							
200							
298	17.060	30.949	30.949	.000	-143.779	-134.789	98.798
300	17.088	31.055	30.949	.032	-143.773	-134.733	98.148
400	18.045	36.123	31.633	1.706	-143.493	-131.768	71.901
500	18.677	40.228	32.955	3.636	-143.108	-128.884	56.332
600	19.090	43.634	34.659	5.505	-142.777	-126.072	45.919
700	22.000	46.807	35.995	7.269	-142.284	-123.321	38.501
800	22.000	49.745	37.534	9.769	-141.695	-120.654	32.959
900	22.000	52.336	39.038	11.969	-141.146	-118.050	28.667
1000	22.000	54.654	40.485	14.169	-140.759	-115.537	25.206
1100	22.000	56.751	41.870	16.369	-140.258	-112.621	22.375
1200	22.000	58.665	43.191	18.569	-141.785	-109.948	20.023
1300	22.000	60.426	44.450	20.769	-141.340	-107.313	18.040
1400	22.000	62.056	45.650	22.969	-171.288	-104.231	16.270
1500	22.000	63.574	46.795	25.169	-170.491	-99.469	14.492
1600	22.000	64.994	47.889	27.369	-169.696	-94.762	12.943
1700	22.000	66.328	48.935	29.569	-168.900	-90.191	11.583
1800	22.000	67.585	49.936	31.769	-168.110	-85.849	10.376
1900	22.000	68.775	50.897	33.969	-167.318	-81.920	9.307
2000	22.000	69.903	51.819	36.169	-166.530	-78.392	8.347
2100	22.000	70.977	52.706	38.369	-165.742	-71.908	7.483
2200	22.000	72.000	53.560	40.569	-164.957	-67.456	6.701
2300	22.000	72.978	54.383	42.769	-164.173	-63.040	5.990
2400	22.000	73.914	55.177	44.969	-163.391	-58.660	5.341
2500	22.000	74.812	55.945	47.169	-162.613	-54.313	4.748
2600	22.000	75.675	56.687	49.369	-161.836	-49.995	4.202
2700	22.000	76.506	57.406	51.569	-161.063	-45.711	3.700
2800	22.000	77.306	58.103	53.769	-160.293	-41.453	3.235
2900	22.000	78.078	58.778	55.969	-159.526	-37.222	2.805
3000	22.000	78.824	59.434	58.169	-158.764	-33.019	2.405

Dec. 31, 1960; Dec. 31, 1965

MAGNESIUM DICHLORIDE (MgCl<sub>2</sub>)

(LIQUID)

MOL. WT. = 95.218

$$S_{298.15}^o = 30.949 \text{ cal. deg.}^{-1} \text{ mole}^{-1}$$

$$\Delta H_f^o 298.15 = -143.779 \text{ kcal. mole}^{-1}$$

$$T_m = 987^{\circ}\text{K.}$$

$$\Delta H_m^o = 10.30 \pm 0.05 \text{ kcal. mole}^{-1}$$

$$T_b = [1710]^{\circ}\text{K.}$$

$$\Delta H_v^o = [37.34] \text{ kcal. mole}^{-1}$$

Heat of Formation.

$\Delta H_f^o 298.15(l)$  was calculated from  $\Delta H_f^o 298.15(c)$  by adding  $\Delta H_m^o$  and the difference between  $H_m^o - H_{298}^o$  for crystal and liquid.

Heat Capacity and Entropy.

A constant  $C_p(l) = 22.0 \text{ cal. deg.}^{-1} \text{ mole}^{-1}$  over the temperature range 1006-1428°K. is from the high temperature heat content data of G. E. Moore, J. Am. Chem. Soc. 65, 1700 (1943). This constant value was assumed to hold from an assumed glass transition of 660°K. to 3000°K.  $C_p(l)$  below 660°K. is taken to be that of the crystal. The entropy was obtained in a manner analogous to the heat of formation.

Melting Data.

See MgCl<sub>2</sub>(c) table for details.

Vaporization Data.

$T_b$  is calculated as the temperature at which the free energy change of the reaction  $\text{MgCl}_2(l) = \text{MgCl}_2(g)$  approaches zero. The difference between  $\Delta H_f^o$  for MgCl<sub>2</sub>(l) and MgCl<sub>2</sub>(g) at  $T_b$  is  $\Delta H_v^o$ .

Cl<sub>2</sub>Mg



## Magnesium (Mg)

(Reference State) At. Wt. = 24.32

T, °K.	cal. mole <sup>-1</sup> deg. <sup>-1</sup>			kcal. mole <sup>-1</sup>			Log K <sub>P</sub>
	C <sub>p</sub>	S°	-(F°-H° <sub>298</sub> )/T	H°-H° <sub>298</sub>	ΔH <sub>f</sub> °	ΔF <sub>f</sub> °	
0	.000	.000	INFINITE	-1.196	.000	.000	.000
100	3.768	2.273	12.695	-1.042	.000	.000	.000
200	5.440	5.533	7.933	.480	.000	.000	.000
298	5.973	7.814	7.814	.000	.000	.000	.000
300	5.960	7.851	7.814	.011	.000	.000	.000
400	6.290	9.613	8.052	.625	.000	.000	.000
500	6.560	11.047	8.512	1.267	.000	.000	.000
600	6.802	12.264	9.036	1.936	.000	.000	.000
700	7.080	13.333	9.577	2.629	.000	.000	.000
800	7.420	14.300	10.108	3.354	.000	.000	.000
900	7.810	15.196	10.624	4.115	.000	.000	.000
1000	7.880	18.339	11.304	7.034	.000	.000	.000
1100	8.140	19.102	11.979	7.836	.000	.000	.000
1200	8.400	19.821	12.602	8.563	.000	.000	.000
1300	8.660	20.504	13.184	9.516	.000	.000	.000
1400	4.968	43.187	14.072	40.760	.000	.000	.000
1500	4.968	43.930	16.025	41.257	.000	.000	.000
1600	4.968	43.850	17.754	41.754	.000	.000	.000
1700	4.968	44.152	19.298	42.251	.000	.000	.000
1800	4.968	44.436	20.687	42.748	.000	.000	.000
1900	4.968	44.704	21.944	43.244	.000	.000	.000
2000	4.969	44.959	23.088	43.741	.000	.000	.000
2100	4.969	45.201	24.136	44.238	.000	.000	.000
2200	4.970	45.433	25.098	44.735	.000	.000	.000
2300	4.972	45.654	25.987	45.232	.000	.000	.000
2400	4.974	45.865	26.811	45.729	.000	.000	.000
2500	4.978	46.068	27.578	46.227	.000	.000	.000
2600	4.983	46.264	28.292	46.725	.000	.000	.000
2700	4.989	46.452	28.962	47.224	.000	.000	.000
2800	4.998	46.633	29.589	47.723	.000	.000	.000
2900	5.009	46.809	30.180	48.223	.000	.000	.000
3000	5.023	46.979	30.737	48.725	.000	.000	.000
3100	5.040	47.144	31.264	49.228	.000	.000	.000
3200	5.060	47.304	31.763	49.733	.000	.000	.000
3300	5.085	47.460	32.235	50.240	.000	.000	.000
3400	5.114	47.613	32.686	50.750	.000	.000	.000
3500	5.148	47.761	33.115	51.263	.000	.000	.000
3600	5.186	47.907	33.524	51.780	.000	.000	.000
3700	5.229	48.050	33.914	52.301	.000	.000	.000
3800	5.278	48.190	34.288	52.826	.000	.000	.000
3900	5.332	48.327	34.646	53.356	.000	.000	.000
4000	5.392	48.463	34.990	53.892	.000	.000	.000
4100	5.457	48.597	35.320	54.435	.000	.000	.000
4200	5.528	48.729	35.638	54.984	.000	.000	.000
4300	5.604	48.860	35.944	55.541	.000	.000	.000
4400	5.686	48.990	36.239	56.105	.000	.000	.000
4500	5.773	49.119	36.524	56.678	.000	.000	.000
4600	5.866	49.247	36.799	57.260	.000	.000	.000
4700	5.964	49.374	37.065	57.851	.000	.000	.000
4800	6.067	49.501	37.323	58.453	.000	.000	.000
4900	6.176	49.627	37.573	59.065	.000	.000	.000
5000	6.289	49.753	37.815	59.688	.000	.000	.000
5100	6.407	49.878	38.050	60.323	.000	.000	.000
5200	6.530	50.004	38.279	60.970	.000	.000	.000
5300	6.658	50.130	38.501	61.629	.000	.000	.000
5400	6.790	50.255	38.715	62.301	.000	.000	.000
5500	6.927	50.381	38.922	62.987	.000	.000	.000
5600	7.069	50.507	39.125	63.687	.000	.000	.000
5700	7.215	50.634	39.325	64.401	.000	.000	.000
5800	7.367	50.760	39.521	65.130	.000	.000	.000
5900	7.523	50.888	39.722	65.875	.000	.000	.000
6000	7.684	51.015	39.912	66.635	.000	.000	.000

Dec. 31, 1960; Sept. 30, 1962

Mg

MAGNESIUM (Mg)

(REFERENCE STATE)

AT. WT. = 24.32

Crystal Below 922°K  
 Liquid 922°K to 1378°K  
 Ideal gas, monatomic above 1378°K

See crystal, liquid, and ideal monatomic gas for details.

Mg



## Magnesium (Mg)

(Crystal) At. Wt. = 24.32

T, °K.	cal. mole <sup>-1</sup> deg. <sup>-1</sup>			kcal. mole <sup>-1</sup>			Log K <sub>F</sub>
	C <sub>p</sub>	S°	-(F°-H° <sub>298</sub> )/T	H°-H° <sub>298</sub>	ΔH <sub>f</sub> °	ΔF <sub>f</sub> °	
0	.000	.000	INFINITE	- 1.196	.000	.000	INFINITE
100	3.768	2.273	12.695	- 1.042	.000	.000	.000
200	5.440	4.533	7.913	-.880	.000	.000	.000
298	5.953	7.814	7.814	.000	.000	.000	.000
300	5.960	7.851	7.814	.011	.000	.000	.000
400	6.290	9.613	8.052	.625	.000	.000	.000
500	6.560	11.047	8.512	1.267	.000	.000	.000
600	6.802	12.264	9.038	1.936	.000	.000	.000
700	7.080	13.393	9.577	2.629	.000	.000	.000
800	7.420	14.300	10.108	3.354	.000	.000	.000
900	7.810	15.197	10.624	4.115	.000	.000	.000
1000	8.190	16.039	11.124	4.915	- 2.119	.181	.040
1100	8.525	16.835	11.607	5.751	- 2.085	.408	-.081
1200	8.860	17.592	12.075	6.620	- 2.043	.633	-.115
1300	9.195	18.314	12.527	7.523	- 1.993	.854	-.144
1400	9.530	19.008	12.965	8.459	- 1.931	1.050	-.162
1500	9.865	19.677	13.391	9.429	- 1.858	1.222	-.176
1600	10.200	20.324	13.804	10.432	- 1.772	1.370	-.183
1700	10.535	20.952	14.206	11.469	- 1.678	1.497	-.183
1800	10.870	21.564	14.598	12.539	- 1.575	1.601	-.173
1900	11.205	22.161	14.980	13.643	- 1.461	1.681	-.152
2000	11.540	22.747	15.354	14.780	- 1.328	1.729	-.119

Dec. 31, 1960; Sept. 30, 1962

Mg

## MAGNESIUM (Mg)

(CRYSTAL)

AT. WT. = 24.32

$$\Delta H_f^0 = 0$$

$$\Delta H_f^{298.15} = 0$$

$$\Delta H_f^{298.15} = 35.28 \pm 0.01 \text{ kcal. mole}^{-1}$$

$$S_{298.15}^0 = 7.814 \text{ cal. deg.}^{-1} \text{ mole}^{-1}$$

$$T_m = 922 \pm 0.5^\circ\text{K}$$

$$\Delta H_m = 2.14 \text{ kcal. mole}^{-1}$$

## Heat of Formation.

Zero by definition.

## Heat Capacity and Entropy.

The following heat capacity measurements were considered in drawing a smooth curve of  $C_p$  with T: P. L. Smith (1.25-4.2°K) Phil. Mag. 46, 744 (1955); J. R. Clement and H. R. Jeffers (3-13°K) Phys. Rev. 105, 1435 (1957); K. Clusius and J. V. Vaughn (11.3-228.4°K) J. Am. Chem. Soc. 52, 4686, (1930); R. S. Craig, C. A. Krier, L. W. Coffey, E. A. Bates, and W. E. Wallace (12-320°K) J. Am. Chem. Soc. 76, 236 (1954); W. Mannchen and K. Bornkessel (190-300°K) Z. Metallkunde 51, 482-5 (1960); H. Seekamp (291-773°K) Z. anorg. Chem. 195, 345 (1931); and D. R. Stull and R. A. McDonald (700-900°K) J. Am. Chem. Soc. 77, 5293 (1955). The following heat capacity measurements were noted but not used as the data were either not tabulated, or erratic, or inconsistent or would not have altered the  $C_p$ -T curve: D. L. Martin (0.4-1.5°K) Proc. Phys. Soc. (London) 78, 1482-8 (1961); I. Estermann, S. A. Friedberg, and J. E. Goldman (1.8-4.2°K) Phys. Rev. 87, 582 (1952); E. P. Eastman and W. H. Rodebush (74.9-288.5°K) J. Am. Chem. Soc. 40, 489 (1918); W. G. Sabs, K. F. Sterrett, R. S. Craig, and W. E. Wallace (298-543°K) J. Am. Chem. Soc. 79, 3637 (1957); F. M. Jaeger and T. J. Foppema (273-873°K) Rec. Trav. chim. 55, 492 (1936); J. H. Awbrey and E. Griffiths (323-898°K) Proc. Phys. Soc. 36, 378 (1926); E. D. Eastman, A. M. Williams and T. P. Young (373-873°K) J. Am. Chem. Soc. 46, 1178 (1926); and F. Schübel (323-773°K) Z. anorg. Chem. 87, 81 (1914).  $S_{298.15}^0$  was obtained by numerical integration using the low temperature  $C_p$  data cited above.

## Melting.

Melting point is from J. L. Haughton and R. J. M. Payne (922 ± 0.5°K) J. Inst. Met. 54, 279 (1954). Also noted but not used were: R. Chadwick (923°K) J. Inst. Met. 39, 285-300 (1928); W. R. D. Jones (920.5°K) J. Inst. Met. 46, 395-419 (1931).

The heat of melting is from D. R. Stull and R. A. McDonald (loc. cit.)

## Heat of Sublimation.

Is obtained by third law calculations from the vapor pressure data on the solid by P. P. Coleman and A. E. Egerton, Phil. Trans. Roy. Soc. (London) A234, 177-204 (1935) and the value is confirmed by similar use of the vapor pressure data on the liquid by E. Scheil and P. Wolf, Z. Metallkunde 50, 229-33 (1959); A. Wejnarth, Tek. Tid. 22, 35-9, 44-8 (1942); A. Schneider and E. K. Stoll, Z. Elektrochem. 47, 519-26 (1941); E. Baur and R. Brunner, Helv. Chim. Acta, 17, 958-69 (1934); and H. Hartmann and R. Schneider, Z. anorg. Chem. 180, 275-83 (1929). Additional data noted but not used on the vapor pressure, as values were not tabulated or they were erratic, of the solid are by J. P. Smith and R. L. Smythe, Acta Metallurgica, 7, 261-7 (1959); A. Suckow, Metallwirtschaft, 15, 64-5 (1936); W. Leitgeb, Metallwirtschaft, 14, 269 (1935); and of the liquid by P. A. Vetter and O. Kubaschewski, Z. Elektrochem. 57, 243 (1953); W. Leitgeb, Z. anorg. Chem. 202, 312 (1931); C. Zwicker, Physica, 8, 246 (1928); O. Ruff and H. Hartmann, Z. anorg. Chem., 133, 29-45 (1924); and J. Johnston, Ind. Eng. Chem., 9, 876 (1917).

Mg

## Magnesium (Mg)

(Liquid) At. Wt. = 24.32

T. °K.	cal. mole <sup>-1</sup> deg. <sup>-1</sup>			kcal. mole <sup>-1</sup>			Log K <sub>p</sub>
	C <sub>p</sub>	S°	-(F°-H° <sub>298</sub> )/T	H°-H° <sub>298</sub>	ΔH <sub>f</sub> °	ΔF <sub>f</sub> °	
0							
100							
200							
298	5.953	10.159	10.159	.000	2.158	1.459	- 1.069
300	5.960	10.196	10.159	.011	2.158	1.455	- 1.060
400	6.290	11.958	10.397	.625	2.158	1.219	- .656
500	6.560	13.392	10.857	1.267	2.158	.986	- .431
600	6.802	14.609	11.383	1.936	2.158	.750	- .273
700	7.080	14.679	11.922	2.630	2.159	.517	- .161
800	7.350	14.642	12.453	3.351	2.155	.282	- .077
900	7.510	14.523	12.958	4.099	2.142	.048	- .012
1000	7.860	14.338	13.495	4.874	.000	.000	.000
1100	8.140	14.102	13.943	5.675	.000	.000	.000
1200	8.400	14.821	14.403	6.502	.000	.000	.000
1300	8.660	20.504	14.886	7.355	.000	.000	.000
1400	8.920	21.155	15.274	8.234	- 30.368	.477	- .074
1500	9.180	21.779	15.687	9.139	- 29.960	2.666	- .388
1600	9.440	22.380	16.086	10.070	- 29.526	4.826	- .659
1700	9.700	22.960	16.474	11.027	- 29.066	6.960	- .895
1800	9.960	23.522	16.850	12.010	- 28.580	9.065	- 1.101
1900	10.220	24.067	17.215	13.019	- 28.067	11.142	- 1.282
2000	10.480	24.598	17.571	14.054	- 27.529	13.192	- 1.442
2100	10.740	24.116	17.918	15.115	- 26.965	15.213	- 1.583
2200	11.000	24.622	18.257	16.202	- 26.375	17.210	- 1.710
2300	11.260	24.116	18.588	17.315	- 25.759	19.178	- 1.822
2400	11.520	24.601	18.912	18.454	- 25.117	21.117	- 1.921
2500	11.780	27.076	19.229	19.619	- 24.450	23.029	- 2.013

Dec. 31, 1960; Sept. 30, 1962

Mg

## MAGNESIUM (Mg)

(LIQUID)

AT. WT. = 24.32

$$\Delta H_f^{\circ} 298.15 = [2.158] \text{ kcal. mole}^{-1}$$

$$S_{298.15}^{\circ} = [10.159] \text{ cal. deg.}^{-1} \text{ mole}^{-1}$$

$$T_m = 922 \pm 0.5^{\circ}\text{K}$$

$$\Delta H_m^{\circ} = 2.140 \text{ cal. mole}^{-1}$$

$$T_b = 1378^{\circ}\text{K}$$

$$\Delta H_v = 30.5 \text{ kcal. mole}^{-1}$$

## Heat of Formation.

$\Delta H_f^{\circ} 298.15$  (=  $\Delta H_m 298.15$ ) obtained from  $\Delta H_m 922$  by adding  $H_{922} - H_{298.15}$  for solid and subtracting  $H_{922} - H_{298.15}$  for liquid.

## Heat Capacity and Entropy.

The heat capacity measurements of D. R. Stull and R. A. McDonald (950-1100°K) J. Am. Chem. Soc. 77, 5293 (1955) were used. Outside of the observed range  $C_p$  was extrapolated linearly with temperature. Below  $T_m$  the linear extrapolation was continued until the  $C_p$  curve for the solid is encountered at 710°K. At lower temperatures the  $C_p$  of the crystal is used.  $S_{298.15}^{\circ}$  was calculated from that of the solid.

## Melting.

See crystal for details.

## Vaporization.

The normal boiling point was calculated by the third law and  $\Delta H_v 298.15$ . This compares with 1377°K computed from the general vapor pressure equation for liquid Mg given on p 221 of Gmelins Handbuch der anorganischen Chemie, System-Nummer 27 (1952), and experimentally determined values: 1376 ± 5°K by A. Schneider and U. Esch, Z. Elektrochem 45, 888 (1953); 1380°K by E. Baur and R. Brunner, Helv. Chim. Acta 17, 958 (1934); 1370°K by W. Leitgeb, Z. anorg. Chem. 202, 305 (1931); and 1393°K by Greenwood, Chem. News 104, 31 (1911).

The  $\Delta H_v 1378$  is based on the liquid and ideal gas tables.

Mg

Magnesium, Monatomic (Mg)  
(Ideal Gas) At. Wt. = 24.32

Mg

T, °K.	cal. mole <sup>-1</sup> deg. <sup>-1</sup>			kcal. mole <sup>-1</sup>			Log K <sub>p</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup>	-(F <sup>o</sup> -H <sub>298<sup>o</sup>})/T</sub>	H <sup>o</sup> -H <sub>298<sup>o</sup></sub>	ΔH <sub>f</sub> <sup>o</sup>	ΔF <sub>f</sub> <sup>o</sup>	
0	4.968	34.520	35.958	1.481	34.996	34.996	INFINITE
100	4.968	34.520	35.958	1.481	34.996	34.996	INFINITE
200	4.968	34.520	35.958	1.481	34.996	34.996	INFINITE
298	4.968	34.504	35.504	1.481	34.996	34.996	INFINITE
300	4.968	34.535	35.504	1.481	34.996	34.996	INFINITE
400	4.968	34.964	35.494	1.481	34.996	34.996	INFINITE
500	4.968	34.972	35.057	1.481	34.996	34.996	INFINITE
600	4.968	34.978	34.479	1.481	34.845	18.816	6.853
700	4.968	34.744	34.892	1.481	34.648	16.161	5.045
800	4.968	34.497	34.291	1.481	34.420	13.534	3.497
900	4.968	34.243	33.670	1.481	34.156	10.939	2.456
1000	4.968	34.016	33.029	1.481	33.734	8.557	1.870
1100	4.968	33.819	32.368	1.481	33.269	6.252	1.242
1200	4.968	33.642	31.688	1.481	32.769	4.027	0.724
1300	4.968	33.482	31.001	1.481	32.232	2.873	0.291
1400	4.968	33.336	30.308	1.481	31.658	1.777	0.000
1500	4.968	33.202	29.609	1.481	31.047	0.727	0.000
1600	4.968	33.078	28.905	1.481	30.398	0.727	0.000
1700	4.968	32.964	28.197	1.481	29.711	0.727	0.000
1800	4.968	32.859	27.484	1.481	28.986	0.727	0.000
1900	4.968	32.762	26.766	1.481	28.223	0.727	0.000
2000	4.969	32.672	26.043	1.481	27.423	0.727	0.000
2100	4.969	32.588	25.315	1.481	26.586	0.727	0.000
2200	4.970	32.509	24.582	1.481	25.712	0.727	0.000
2300	4.972	32.435	23.844	1.481	24.801	0.727	0.000
2400	4.974	32.365	23.101	1.481	23.852	0.727	0.000
2500	4.978	32.300	22.353	1.481	22.865	0.727	0.000
2600	4.983	32.241	21.600	1.481	21.839	0.727	0.000
2700	4.989	32.188	20.842	1.481	20.773	0.727	0.000
2800	4.998	32.140	20.079	1.481	19.667	0.727	0.000
2900	5.009	32.097	19.311	1.481	18.521	0.727	0.000
3000	5.023	32.059	18.538	1.481	17.335	0.727	0.000
3100	5.040	32.025	17.760	1.481	16.109	0.727	0.000
3200	5.060	32.000	16.977	1.481	14.943	0.727	0.000
3300	5.085	32.000	16.190	1.481	13.837	0.727	0.000
3400	5.114	32.000	15.400	1.481	12.791	0.727	0.000
3500	5.148	32.000	14.607	1.481	11.805	0.727	0.000
3600	5.186	32.000	13.811	1.481	10.879	0.727	0.000
3700	5.229	32.000	13.014	1.481	10.013	0.727	0.000
3800	5.278	32.000	12.214	1.481	9.206	0.727	0.000
3900	5.332	32.000	11.411	1.481	8.458	0.727	0.000
4000	5.392	32.000	10.604	1.481	7.769	0.727	0.000
4100	5.457	32.000	9.793	1.481	7.139	0.727	0.000
4200	5.528	32.000	8.977	1.481	6.567	0.727	0.000
4300	5.604	32.000	8.156	1.481	6.053	0.727	0.000
4400	5.686	32.000	7.329	1.481	5.596	0.727	0.000
4500	5.773	32.000	6.496	1.481	5.195	0.727	0.000
4600	5.866	32.000	5.659	1.481	4.849	0.727	0.000
4700	5.964	32.000	4.816	1.481	4.558	0.727	0.000
4800	6.067	32.000	3.967	1.481	4.322	0.727	0.000
4900	6.176	32.000	3.112	1.481	4.140	0.727	0.000
5000	6.289	32.000	2.251	1.481	4.013	0.727	0.000
5100	6.407	32.000	1.384	1.481	3.940	0.727	0.000
5200	6.530	32.000	0.511	1.481	3.921	0.727	0.000
5300	6.658	32.000	-0.366	1.481	3.956	0.727	0.000
5400	6.790	32.000	-1.247	1.481	4.045	0.727	0.000
5500	6.927	32.000	-2.132	1.481	4.188	0.727	0.000
5600	7.069	32.000	-3.021	1.481	4.385	0.727	0.000
5700	7.215	32.000	-3.914	1.481	4.636	0.727	0.000
5800	7.367	32.000	-4.811	1.481	4.941	0.727	0.000
5900	7.523	32.000	-5.712	1.481	5.300	0.727	0.000
6000	7.684	32.000	-6.617	1.481	5.713	0.727	0.000

Dec. 31, 1960; Sept. 30, 1962

MAGNESIUM, MONATOMIC (Mg)

(IDEAL GAS)

AT. WT. = 24.32

$$\Delta H_f^o = 35.0 \pm 0.01 \text{ kcal. mole}^{-1}$$

$$\Delta H_f^o 298.15 = 35.28 \pm 0.01 \text{ kcal. mole}^{-1}$$

Ground State <sup>1</sup>S<sub>0</sub>

$$S_{298.15}^o = 35.504 \text{ cal. mole}^{-1} \text{ deg.}^{-1}$$

Electronic Levels and Multiplicities

E <sub>i</sub> , cm. <sup>-1</sup>	E <sub>i</sub>	E <sub>i</sub> , cm. <sup>-1</sup>	E <sub>i</sub>	E <sub>i</sub> , cm. <sup>-1</sup>	E <sub>i</sub>
0.00	1	46403.14	5	57020	9
21850.37	1	47850.0	9	57204	28
21870.43	3	47957.0	15	57854	12
21911.14	5	48346.6	3	58469	58
35051.56	3	51872.4	3	59315	51
41197.37	3	52556.4	1	59876	51
43503.0	1	53134.7	5	60397	102
				60887	154

Heat of Formation.

ΔH<sub>f</sub><sup>o</sup> 298.15 (=ΔH<sub>f</sub> 298.15) is calculated as described on the table for crystal.

Heat Capacity and Entropy.

Thermodynamic functions were calculated using electronic levels and multiplicities from C. E. Moore [Nat'l. Bur. Standards Circ. 467, Vol. 1 (1949)]. Higher levels were averaged.

Mg