

REFERENCE STATE

0 to 923 K crystal
 923 to 1366.104 K liquid
 above 1366.104 K ideal monatomic gas

Refer to the individual tables for details.

Magnesium (Mg)

Mg₁(ref)

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^o	S° - [C _p ^o - R ln(T _r)]/T	H° - H°(T _r)	ΔG°	
	J·K ⁻¹ ·mol ⁻¹	J·K ⁻¹ ·mol ⁻¹	KJ·mol ⁻¹	KJ·mol ⁻¹	
0	0	INFINITE	-4.998	0	0
100	15.762	9.505	-3.046	0	0
200	22.724	23.143	-2.349	0	0
298.15	24.869	32.671	0	0	0
300	24.897	32.671	0.046	0	0
400	26.144	40.167	2.601	0	0
500	27.171	46.113	5.268	0	0
600	28.184	51.156	8.035	0	0
700	29.279	55.581	10.907	0	0
800	30.507	59.569	13.895	0	0
900	31.895	63.241	17.014	0	0
923.000	32.238	64.050	17.751	0	0
923.000	34.309	75.234	26.228	0	0
1000	34.309	75.983	28.870	0	0
1100	34.309	79.253	32.301	0	0
1200	34.309	82.238	35.732	0	0
1300	34.309	84.984	39.163	0	0
1366.104	34.309	86.686	41.431	0	0
1366.104	20.786	180.286	169.298	0	0
1400	20.786	180.796	170.003	0	0
1500	20.786	182.230	172.082	0	0
1600	20.786	183.571	174.160	0	0
1700	20.786	184.832	176.239	0	0
1800	20.787	186.020	178.317	0	0
1900	20.787	187.144	180.396	0	0
2000	20.789	188.210	182.475	0	0
2100	20.791	189.224	184.554	0	0
2200	20.795	190.192	186.633	0	0
2300	20.802	191.116	188.713	0	0
2400	20.812	192.002	190.794	0	0
2500	20.826	192.851	192.875	0	0
2600	20.846	193.669	194.959	0	0
2700	20.874	194.456	197.045	0	0
2800	20.909	195.216	199.134	0	0
2900	20.956	195.950	201.227	0	0
3000	21.014	196.661	203.326	0	0
3100	21.085	197.352	205.430	0	0
3200	21.172	198.025	207.543	0	0
3300	21.272	198.678	209.665	0	0
3400	21.389	199.312	211.799	0	0
3500	21.537	199.934	213.945	0	0
3600	21.697	200.543	216.107	0	0
3700	21.879	201.140	218.285	0	0
3800	22.083	201.726	220.483	0	0
3900	22.310	202.303	222.703	0	0
4000	22.559	202.871	224.946	0	0
4100	22.832	203.431	227.215	0	0
4200	23.128	203.985	229.513	0	0
4300	23.447	204.533	231.842	0	0
4400	23.789	205.076	234.203	0	0
4500	24.152	205.614	236.600	0	0
4600	24.537	206.149	239.034	0	0
4700	24.944	206.681	241.508	0	0
4800	25.372	207.211	244.023	0	0
4900	25.820	207.739	246.583	0	0
5000	26.287	208.265	249.188	0	0
5100	26.773	208.790	251.841	0	0
5200	27.276	209.315	254.543	0	0
5300	27.794	209.839	257.296	0	0
5400	28.329	210.364	260.102	0	0
5500	28.878	210.888	262.962	0	0
5600	29.442	211.414	265.878	0	0
5700	30.020	211.940	268.851	0	0
5800	30.610	212.467	271.882	0	0
5900	31.213	212.996	274.973	0	0
6000	31.827	213.525	278.125	0	0

PREVIOUS September 1982 (1 atm)

CURRENT September 1983 (1 bar)

Magnesium (Mg)

Mg₁(ref)

Mg₁(cr)

Magnesium (Mg)

A₁ = 24.3057

CRYSTAL

Magnesium (Mg)

Pearson Notation: hF2
 $S^{\circ}(298.15 \text{ K}) = 32.671 \pm 0.10 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $T_{\text{fus}} = 923 \pm 1 \text{ K}$
 $\Delta H_f^{\circ}(0 \text{ K}) = 0 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta H_f^{\circ}(298.15 \text{ K}) = 0 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{fus}}H^{\circ}(923 \text{ K}) = 8.477 \pm 0.418 \text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The adopted heat capacities are derived from heat capacity² and enthalpy data³ by fitting the experimental data with orthogonal polynomials over selected overlapping temperature intervals. The temperature region of 114 K is described by the equation $C_p^{\circ} = 0.3 \times 10^{-4} T + 0.8 \times 10^{-6} T^2 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$. The $S^{\circ}(298.15 \text{ K})$ value calculated from the polynomials agrees with those of Hultgren *et al.*,⁴ Gurvich *et al.*,⁵ and CODATA⁶ to within $0.01 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.

Craig *et al.*¹ measured the heat capacity in the region 12–320 K. Only smoothed values at 10 K intervals were reported and these were based on an incorrect relative atomic mass. Furukawa *et al.*⁴ stated that the heat capacity values should be multiplied by 24.32/24.22 = 1.0041 to be consistent with the atomic mass of 1954. The current value for the relative atomic mass of magnesium requires a multiplier of 24.305/24.22 = 1.0035. Our analysis of this smoothed data (with orthogonal polynomials) suggests that the reported values at 18 K and 200 K may be in error.

The heat capacity study of Saba *et al.*² consisted of 37 determinations covering the range 293–548 K. Again only smoothed values at 10 K intervals were given. Using the current relative atomic mass for magnesium, this data should be multiplied by 24.305/24.32 = 0.99938. The enthalpy data of McDonald,³ 6 values in the range 404–914 K, also need to be corrected by a factor of 24.305/24.312 = 0.99971. In the region 300–320 K, the corrected results of Craig *et al.*¹ lie 0.1% higher and Saba *et al.*² 0.2% lower than the adopted values. The maximum deviation in the enthalpy data of McDonald³ in comparison with our derived enthalpy values is 0.1%, except for the point at 403 K which is 0.7%. At the melting point, the entropies of JANAF,⁷ Hultgren *et al.*,⁴ and Gurvich *et al.*⁵ are 15.308, 15.34, and 15.313 cal $\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$, respectively.

Other studies^{8–11} are considered for comparison with and confirmation of the adopted values, but they are not included in the polynomial fitting procedure. The heat capacity results of Mannchen and Bornkessel,⁸ 12–300 K, were presented only graphically and support the results of Craig *et al.*¹ The quantitative agreement is uncertain since it is not clear if the authors⁸ were aware of the correction required for the data of Craig *et al.*¹ Clusius and Vaughn⁹ made experimental heat capacity determinations in the range 11–228 K. These data scatter about the selected values within ± 2 –4%.

Phase Data

According to Pearson,¹⁵ magnesium has the hcp(A3) prototype structure. In the alkaline earth metal series, only α -Be has a similar structure.

Fusion Data

Refer to the liquid table for details.

Sublimation Data

The enthalpy of sublimation of magnesium is the enthalpy of formation of the gas. It is chosen to be that adopted by CODATA⁶ based on numerous experimental studies which are discussed in the ideal gas table.¹⁴

References

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Mg₁(cr)

Magnesium (Mg)

PREVIOUS: September 1962

CURRENT: September 1983

Magnesium (Mg) $A_r = 24.305$ Magnesium (Mg) $Mg(l)$

T/K	C _p ^a	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K _f
		S° - [G° - H°(T _r)]/T	H° - H°(T _r)	Δ _{sub} H°	Δ _{sub} G°	
0						
100						
200						
250						
298.15	34.309	34.464	0.	4.790	4.256	-0.746
300	34.309	34.676	0.063	4.808	4.252	-0.740
350	34.309	39.965	34.882	5.261	4.124	-0.615
400	34.309	44.546	35.810	5.684	3.932	-0.513
450	34.309	48.587	37.010	6.078	3.689	-0.428
500	34.309	52.202	38.352	6.448	3.403	-0.356
600	34.309	58.457	41.197	7.111	2.731	-0.238
700	34.309	63.746	44.050	7.670	1.955	-0.126
800	34.309	68.327	46.805	8.113	1.107	-0.072
900	34.309	72.368	49.425	8.425	0.211	-0.012
923.000	34.309	73.234	50.008	21.438	0.	0.
1000	34.309	75.983	51.903	24.080	0.	0.
1100	34.309	79.253	54.243	27.511	0.	0.
1200	34.309	82.238	56.854	30.741	0.	0.
1300	34.309	84.984	58.544	34.372	0.	0.
1366.104	34.309	86.686	59.865	36.640	---	---
1400	34.309	87.527	60.525	37.803	3.167	-0.118
1500	34.309	89.894	62.405	41.234	12.447	-0.433
1600	34.309	92.108	64.193	44.665	21.636	-0.706
1700	34.309	94.188	65.871	48.076	30.741	-0.945
1800	34.309	96.149	67.425	51.352	39.765	-1.154
1900	34.309	98.004	69.079	54.538	48.717	-1.339
2000	34.309	99.764	70.570	58.388	57.596	-1.504

Magnesium (Mg) $S^{\circ}(298.15\text{ K}) = [34.464] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ $\Delta_{\text{sub}}H^{\circ}(298.15\text{ K}) = [4.790] \text{ kJ}\cdot\text{mol}^{-1}$
 $T_{\text{m}} = 923 \pm 1 \text{ K}$ $\Delta_{\text{sub}}H^{\circ}(923\text{ K}) = 8.477 \pm 0.418 \text{ kJ}\cdot\text{mol}^{-1}$

LIQUID

Enthalpy of Formation
 The heat of formation is calculated from that of the crystal by addition of the heat of fusion, $\Delta_{\text{sub}}H^{\circ}(923\text{ K})$, and the enthalpy differences, $H^{\circ}(923;298.15)$, for the crystal and the liquid. This value is dependent on the arbitrary choice of the liquid phase heat capacity values for temperatures less than 923 K.

Heat Capacity and Entropy
 The enthalpy measurements of McDonald,¹ five observations in the temperature range 954–1263 K, are used to derive a constant liquid phase heat capacity of $8.2 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$. This constant value is adopted for the entire liquid region and the region between 298.15 and 923 K. Gurvich *et al.*¹³ have adopted the same value. Kubaschewski² quoted an unpublished study by Reinartz which gave $C_p^{\circ}(l) = 8.1 \pm 0.3 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$. The enthalpies measured by McDonald deviate by -0.2 to +0.3% from the adopted values. The enthalpy study of Awbery and Griffiths³ extended only 100 K into the liquid region (3 data points) and cannot be used to reliably predict the heat capacity; in addition, their reported enthalpies are 15% lower than the adopted values.

Fusion Data
 The melting point is adopted as $923 \pm 1 \text{ K}$. Charlesworth⁴ and Geschneider⁵ both adopted this value after critically reviewing the available data in 1964 and 1970, respectively. The primary studies are by Chadwick⁶ (923 K), Jones⁷ (920.5 K), and Haughton and Payne⁸ (922 ± 0.5 K).

The adopted heat of melting, $\Delta_{\text{sub}}H^{\circ} = 2.026 \text{ kcal}\cdot\text{mol}^{-1}$, is derived from the enthalpy study of McDonald.¹ Although McDonald¹ reports an uncertainty of ±50 cal·mol⁻¹, we feel a value of ±100 cal·mol⁻¹ reflects better the scatter of the various studies. Kubaschewski² quoted values for $\Delta_{\text{sub}}H^{\circ}$ of 2.030 ± 0.080 and 1.830 ± 0.090 kcal·mol⁻¹ from the unpublished work of Reinartz and a thesis of Witting, respectively. The calorimetric studies of Ginsberg and Wrigge⁹ and the DTA study of Chioiti *et al.*¹⁰ led to values of $90.6 \pm 2 \text{ cal/g}$ (2.202 ± 0.049 kcal·mol⁻¹) and $1.970 \pm 0.016 \text{ kcal}\cdot\text{mol}^{-1}$, respectively. An enthalpy study of Succitruill and McDonald¹¹ led to a heat of melting of 2.14 kcal·mol⁻¹; however, this value was thought to be in error due to a container reaction. These reported values all support the adopted value. The enthalpy study of Awbery and Griffiths³ led to a much lower value of 1.130 kcal·mol⁻¹.

Vaporization Data
 T_b is calculated as the temperature for which $\Delta_{\text{sub}}G^{\circ} = 0$ for the liquid vaporizing to the ideal monatomic gas. T_b corresponds to a fugacity of one bar. The heat of vaporization is calculated from the heat of formation of the liquid and the gas at T_b . Vaporization studies are discussed in the Mg(g) single phase table.¹²

References
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¹¹D. R. Stull and R. A. McDonald, *J. Amer. Chem. Soc.* **77**, 5293 (1955).
¹²JANAF Thermochemical Tables: Mg(g), 3-31-82.
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CRYSTAL-LIQUID

Magnesium (Mg)

0 to 923 K crystal
above 923 K liquid

Refer to the individual tables for details.

Magnesium (Mg)

Mg (cr,l)

Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa				
T/K	C_p°	$S^\circ - [C_p^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K _r
		$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	
0	0	INFINITE	0	0	0	0
100	15.762	9.505	-4.998	0	0	0
200	22.724	23.145	-4.356	0	0	0
250	24.018	28.364	-2.349	0	0	0
298.15	24.869	32.671	-1.178	0	0	0
300	24.897	32.671	0	0	0	0
350	25.568	36.715	0.046	0	0	0
400	26.144	40.167	1.308	0	0	0
450	26.668	43.277	2.601	0	0	0
500	27.171	46.113	3.922	0	0	0
600	28.184	51.156	5.268	0	0	0
700	29.279	55.281	8.035	0	0	0
800	30.507	59.569	10.907	0	0	0
900	31.895	63.241	13.895	0	0	0
923.000	32.238	64.050	17.751	0	0	0
923.000	34.309	73.234	26.228	0	0	0
1000	34.309	75.983	28.870	0	0	0
1100	34.309	79.253	32.301	0	0	0
1200	34.309	82.238	35.732	0	0	0
1300	34.309	84.984	39.163	0	0	0
1366.104	34.309	86.686	41.431	0	0	0
1400	34.309	87.527	42.594	-127.409	3.167	-0.118
1500	34.309	89.894	46.024	-126.057	12.447	-0.433
1600	34.309	92.108	49.455	-124.705	21.636	-0.706
1700	34.309	94.188	52.886	-123.352	30.741	-0.945
1800	34.309	96.149	56.317	-122.000	39.766	-1.154
1900	34.309	98.004	59.748	-120.648	48.717	-1.339
2000	34.309	99.764	63.179	-119.296	57.596	-1.504

CRYSTAL \leftrightarrow LIQUID TRANSITION

FUGACITY = 1 bar

PREVIOUS:

CURRENT: September 1983

Magnesium (Mg)

Mg(cr,l)

Mg₁(g)

Magnesium (Mg)

IDEAL GAS

Magnesium (Mg)

IP(Mg, g) = 61671.02 ± 0.10 cm⁻¹
 S^o(298.15 K) = 148.648 ± 0.020 J·K⁻¹·mol⁻¹

Δ_rH^o(0 K) = 145.90 ± 0.80 kJ·mol⁻¹
 Δ_rH^o(298.15 K) = 147.10 ± 0.80 kJ·mol⁻¹

A_r = 24.305 Magnesium (Mg)

Electronic Levels and Quantum Weights	g _i
State	ε _i , cm ⁻¹
	0.00
³ S ₀	1
³ P ₀	21850.405
³ P ₁	21870.464
³ P ₂	21911.178
¹ P ₁	35051.264

Enthalpy of Formation

The adopted enthalpy of formation values for Mg(g), Δ_rH^o(298.15 K) = 147.10 ± 0.80 kJ mol⁻¹, is that recommended by CODATA.¹ This value was calculated, according to CODATA, from the vapor pressure measurements by Priselkov (673–773 K),² Gilbreath (495–658 K),³ McCreey and Thom (716–800 K),⁴ Pahlman and Smith (650–930 K),⁵ and others cited in Hultgren *et al.*⁶

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Martin and Zalubas,⁷ is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of fitting in these missing levels (for n < 60) and cutting off the summation in the partition function⁸ has no effect on the thermodynamic functions to 4000 K. This is a result of the high energy of all levels other than the ground state and the levels listed above; the next excited state is approximately 41197 cm⁻¹ above the ground state. Although we list only a few levels, all levels listed by Martin and Zalubas⁷ and estimated levels (for n < 60) are considered in the calculation. The reported uncertainty in S^o(298.15 K) is due to uncertainties in the relative atomic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the additional states and use of different fill and cutoff procedures.⁸

The thermal functions at 298.15 K differ from the CODATA recommendations¹ for two reasons. First, the entropy differs by 0.1094 J·K⁻¹·mol⁻¹ because this table uses a reference pressure of 1 bar, whereas CODATA recommendations are based on 1 atm. Second, small changes, ~0.002 J·K⁻¹·mol⁻¹, arise due to the use of slightly different values for the fundamental constants.

References

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T/K	C _p ^o	S ^o - [G ^o - H ^o (T)]/T	Standard State Pressure = P ^o = 0.1 MPa		log K _r
			Enthalpy Reference Temperature = T _r = 298.15 K	Δ _r G ^o	
	J·K ⁻¹ ·mol ⁻¹	J·K ⁻¹ ·mol ⁻¹	H ^o - H ^o (T)	kJ·mol ⁻¹	
0	0	0	-6.197	145.901	INFINITE
100	20.786	125.940	-4.119	135.694	-70.879
200	20.786	140.348	-2.040	123.968	-32.377
250	20.786	144.986	-1.001	118.122	-24.680
298.15	20.786	148.648	0	112.522	-19.713
300	20.786	148.776	0.038	112.307	-19.554
350	20.786	151.980	1.078	106.527	-15.898
400	20.786	154.756	2.117	100.780	-13.161
450	20.786	157.204	3.156	95.067	-11.053
500	20.786	159.394	4.196	89.387	-9.338
600	20.786	163.184	6.274	78.122	-6.801
700	20.786	166.388	8.353	64.546	-4.998
800	20.786	169.164	10.431	49.661	-3.654
900	20.786	171.612	12.510	34.562	-2.615
1000	20.786	173.802	14.589	19.219	-1.828
1100	20.786	175.783	16.667	3.866	-1.201
1200	20.786	177.592	18.746	-13.014	-0.683
1300	20.786	179.255	20.824	-28.762	-0.249
1366.104	20.786	180.286	22.199	---	---
1400	20.786	180.796	22.903	0	0
1500	20.786	182.230	24.982	0	0
1600	20.786	183.571	27.060	0	0
1700	20.786	184.832	29.139	0	0
1800	20.787	186.020	31.218	0	0
1900	20.787	187.144	33.296	0	0
2000	20.789	188.210	35.375	0	0
2100	20.791	189.224	37.454	0	0
2200	20.795	190.192	39.533	0	0
2300	20.802	191.116	41.613	0	0
2400	20.812	192.002	43.694	0	0
2500	20.826	192.851	45.776	0	0
2600	20.846	193.669	47.859	0	0
2700	20.874	194.456	49.945	0	0
2800	20.909	195.216	52.034	0	0
2900	20.956	195.950	54.127	0	0
3000	21.014	196.661	56.226	0	0
3100	21.085	197.352	58.331	0	0
3200	21.172	198.022	60.443	0	0
3300	21.275	198.675	62.566	0	0
3400	21.396	199.312	64.699	0	0
3500	21.537	199.934	66.845	0	0
3600	21.697	200.543	69.007	0	0
3700	21.879	201.140	71.186	0	0
3800	22.083	201.726	73.384	0	0
3900	22.310	202.303	75.603	0	0
4000	22.559	202.871	77.846	0	0
4100	22.832	203.431	80.116	0	0
4200	23.128	203.985	82.413	0	0
4300	23.447	204.533	84.742	0	0
4400	23.789	205.076	87.103	0	0
4500	24.152	205.614	89.500	0	0
4600	24.537	206.149	91.934	0	0
4700	24.944	206.681	94.408	0	0
4800	25.372	207.211	96.923	0	0
4900	25.820	207.739	99.483	0	0
5000	26.287	208.265	102.088	0	0
5100	26.773	208.790	104.741	0	0
5200	27.276	209.315	107.443	0	0
5300	27.794	209.839	110.196	0	0
5400	28.329	210.364	113.002	0	0
5500	28.878	210.888	115.862	0	0
5600	29.442	211.414	118.778	0	0
5700	30.020	211.940	121.751	0	0
5800	30.610	212.467	124.782	0	0
5900	31.213	212.996	127.873	0	0
6000	31.827	213.525	131.025	0	0

PREVIOUS: September 1963 (1 atm) CURRENT: September 1983 (1 bar)

Magnesium (Mg)

Mg₁(g)

IDEAL GAS

Magnesium, Ion (Mg⁺)

Magnesium, Ion (Mg⁺)

Mg²⁺(g)

IP(Mg⁺, g) = 121267.61 ± 0.05 cm⁻¹
 S^o(298.15 K) = 154.410 ± 0.02 J·K⁻¹·mol⁻¹

Δ_fH^o(0 K) = 883.65 ± 1.3 kJ·mol⁻¹
 Δ_fH^o(298.15 K) = [891.047] kJ·mol⁻¹

Electronic Levels and Quantum Weights	ε _n , cm ⁻¹	g _n
State		
² S _{1/2}	0.00	2
² P _{1/2}	35669.31	2
² P _{3/2}	35760.88	4

Enthalpy of Formation

Δ_fH^o(Mg⁺, g, 0 K) is calculated from Δ_fH^o(Mg, g, 0 K) using the spectroscopic value of IP(Mg) = 61671.02 ± 0.10 cm⁻¹ (737.749 ± 0.001 kJ·mol⁻¹) from Martin and Zolubas.² The ionization limit is converted from cm⁻¹ to kJ mol⁻¹ using the factor, 1 cm⁻¹ = 0.01196266 kJ·mol⁻¹, which is derived from the 1973 CODATA fundamental constants.³ Rosenstock *et al.*,⁴ and Levin and Lias⁵ have summarized additional ionization and appearance potential data.

Δ_fH^o(Mg⁺, g, 298.15 K) is calculated from Δ_fH^o(Mg, g, 0 K) by using IP(Mg) with JANAF¹ enthalpies, H^o(0 K) - H^o(298.15 K), for Mg(g), Mg⁺(g), and e⁻(ref). Δ_fH^o(Mg → Mg⁺ + e⁻, 298.15 K) differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*,⁴ Δ_fH^o(298.15 K) should be changed by -6.197 kJ·mol⁻¹ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Martin and Zolubas,² is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function⁶ has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state and the first two excited states, the next excited state is 69804.95 cm⁻¹ above the ground state. Since inclusion of these higher excited states has no effect on the thermodynamic functions (to 6000 K), we list only the ground state and the first two excited states. The reported uncertainty in S^o(298.15 K) is due to uncertainties in the relative ionic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the excited states and use of different fill and cutoff procedures.⁶

References

- ¹JANAF Thermochemical Tables: Mg(g), 9-30-83; e⁻(ref), 3-31-82.
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- ³E. R. Cohen and B. N. Taylor, *J. Phys. Chem. Ref. Data* 2, 663 (1973).
- ⁴H. M. Rosenstock, K. Draxl, *et al.*, *J. Phys. Chem. Ref. Data* 6, Supp. 1 (1977).
- ⁵R. D. Levin and S. G. Lias, *U. S. Nat. Bur. Stand., NSRDS-NBS-71*, (1982).
- ⁶J. R. Downey, Jr., The Dow Chemical Company, AFOSRS-TR-78-0960, Contract No. F44620-75-1-0048, (1978).

T/K	C _p ^o	S ^o - (G ^o - F(T))/T	H ^o - H ^o (T)	Δ _f H ^o	log K _r
0	0	INFINITE	-6.197	883.650	-148.653
100	20.786	131.703	-1.119	891.047	-147.690
200	20.786	146.111	-2.040	891.047	-147.690
250	20.786	150.749	-1.001	891.047	-147.690
298.15	20.786	154.410	0	891.047	-147.690
300	20.786	154.539	0.038	891.047	-147.690
350	20.786	157.743	1.078	891.047	-147.690
400	20.786	160.519	2.117	891.047	-147.690
450	20.786	162.967	3.156	891.047	-147.690
500	20.786	165.157	4.196	891.047	-147.690
600	20.786	168.947	6.274	891.047	-147.690
700	20.786	172.151	8.353	891.047	-147.690
800	20.786	174.926	10.431	891.047	-147.690
900	20.786	177.375	12.510	891.047	-147.690
1000	20.786	179.565	14.589	891.047	-147.690
1100	20.786	181.546	16.667	891.047	-147.690
1200	20.786	183.354	18.746	891.047	-147.690
1300	20.786	185.018	20.824	891.047	-147.690
1400	20.786	186.559	22.903	891.047	-147.690
1500	20.786	188.000	24.982	891.047	-147.690
1600	20.786	189.334	27.060	891.047	-147.690
1700	20.786	190.594	29.139	891.047	-147.690
1800	20.786	191.783	31.217	891.047	-147.690
1900	20.786	192.906	33.296	891.047	-147.690
2000	20.786	193.973	35.375	891.047	-147.690
2100	20.786	194.987	37.453	891.047	-147.690
2200	20.786	195.954	39.532	891.047	-147.690
2300	20.786	196.878	41.610	891.047	-147.690
2400	20.786	197.762	43.689	891.047	-147.690
2500	20.786	198.611	45.768	891.047	-147.690
2600	20.786	199.426	47.846	891.047	-147.690
2700	20.786	200.211	49.925	891.047	-147.690
2800	20.786	200.966	52.004	891.047	-147.690
2900	20.786	201.696	54.082	891.047	-147.690
3000	20.786	202.401	56.161	891.047	-147.690
3100	20.786	203.082	58.239	891.047	-147.690
3200	20.787	203.742	60.318	891.047	-147.690
3300	20.787	204.382	62.397	891.047	-147.690
3400	20.788	205.002	64.475	891.047	-147.690
3500	20.788	205.605	66.554	891.047	-147.690
3600	20.789	206.191	68.633	891.047	-147.690
3700	20.790	206.760	70.712	891.047	-147.690
3800	20.792	207.315	72.791	891.047	-147.690
3900	20.794	207.855	74.871	891.047	-147.690
4000	20.797	208.381	76.950	891.047	-147.690
4100	20.800	208.895	79.030	891.047	-147.690
4200	20.804	209.396	81.110	891.047	-147.690
4300	20.809	209.886	83.191	891.047	-147.690
4400	20.815	210.364	85.272	891.047	-147.690
4500	20.822	210.832	87.354	891.047	-147.690
4600	20.830	211.290	89.436	891.047	-147.690
4700	20.839	211.738	91.520	891.047	-147.690
4800	20.850	212.177	93.604	891.047	-147.690
4900	20.862	212.607	95.690	891.047	-147.690
5000	20.876	213.028	97.777	891.047	-147.690
5100	20.892	213.442	99.865	891.047	-147.690
5200	20.910	213.848	101.955	891.047	-147.690
5300	20.930	214.246	104.047	891.047	-147.690
5400	20.952	214.638	106.141	891.047	-147.690
5500	20.976	215.022	108.238	891.047	-147.690
5600	21.003	215.400	110.337	891.047	-147.690
5700	21.032	215.772	112.438	891.047	-147.690
5800	21.063	216.138	114.543	891.047	-147.690
5900	21.098	216.499	116.651	891.047	-147.690
6000	21.134	216.854	118.763	891.047	-147.690

PREVIOUS December 1970 (1 atm)

CURRENT September 1983 (1 bar)

IDEAL GAS

Magnesium Nitride (MgN)

Mg₂N₃(g)

Mg₂N₃(g)

$S^{\circ}(298.15\text{ K}) = [224.835] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $\Delta H_f^{\circ}(0\text{ K}) = [289.04 \pm 25.1] \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta H_f^{\circ}(298.15\text{ K}) = [288.70 \pm 25.1] \text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum State	Weight <i>g_i</i>
[¹ Π]	0
$\omega_e = [700] \text{ cm}^{-1}$	
$B_e = [0.5542] \text{ cm}^{-1}$	
$\omega_e x_e = [4.8] \text{ cm}^{-1}$	$\sigma = 1$
$\alpha_e = [0.0052] \text{ cm}^{-1}$	$r_e = [1.85] \text{ \AA}$

Enthalpy of Formation

$\Delta H_f^{\circ}(\text{MgN}, g, 298.15\text{ K})$ was estimated from bond strengths using MgO and comparison with analogous pairs of compounds such as, PN and PO, and also the bond strengths of C-N and C-O in organic compounds.

Heat Capacity and Entropy

The r_e value for MgN was estimated from MgO by comparison with similar pairs PO and PN, SiO and SiN, and AlO and AlN. Using Guggenheimer,¹ ω for MgO was found to lie between the single and multiple bonding cases. Magnesium nitride was assumed to be similar to MgO and ω_e , 700 cm^{-1} was obtained. It was assumed that the $x_e \mu^{1/2}$ value for MgN was equal to that for MgO thus giving $\omega_e x_e = 4.8 \text{ cm}^{-1}$. B_e was calculated from r_e . The α_e value was calculated from B_e , ω_e , and $\omega_e x_e$.

Reference

¹Guggenheimer's Relation, Proc. Phys. Soc. (London) 58, 456 (1946).

T/K	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^{\circ} = 0.1\text{ MPa}$		log K _r
	C_p°	$S^{\circ} - (G^{\circ} - H_f^{\circ}(T_r))/T$	$H^{\circ} - H_f^{\circ}(T)$	ΔG°	
0	0	0	INFINITE	289.040	INFINITE
100	29.151	191.683	252.482	279.629	-146.063
200	30.587	212.211	227.762	269.548	-70.999
250	31.725	219.159	225.368	264.634	-55.292
298.15	32.733	224.835	224.835	259.966	-45.545
300	32.768	225.037	0.061	259.788	-45.233
350	33.639	230.156	225.238	249.729	-38.656
400	34.480	234.996	226.141	240.256	-32.303
450	35.301	238.774	227.222	231.533	-26.303
500	35.530	242.475	228.655	224.886	-20.165
600	36.013	248.983	231.516	216.694	-12.606
700	36.468	254.570	234.420	210.536	-6.606
800	36.797	259.463	237.251	205.047	-3.943
900	37.045	263.812	239.965	200.660	-1.878
1000	37.241	267.725	242.548	196.614	-10.270
1100	37.401	271.282	245.001	188.914	-8.971
1200	37.536	274.543	247.329	181.337	-7.893
1300	37.653	277.552	249.540	173.873	-6.986
1400	37.756	280.346	251.642	169.682	-6.331
1500	37.849	282.954	253.643	161.702	-5.979
1600	37.935	285.400	255.552	153.725	-5.672
1700	38.014	287.702	257.376	145.751	-5.400
1800	38.089	289.877	259.122	137.779	-5.159
1900	38.159	291.938	260.795	129.809	-4.943
2000	38.227	293.897	262.402	121.843	-4.749
2100	38.292	295.764	263.947	113.878	-4.574
2200	38.355	297.547	265.434	105.918	-4.414
2300	38.417	299.253	266.867	97.960	-4.269
2400	38.477	300.889	268.251	89.994	-4.135
2500	38.535	302.461	269.588	82.183	-4.013
2600	38.593	303.974	270.882	74.509	-3.900
2700	38.649	305.431	272.134	66.969	-3.795
2800	38.705	306.838	273.349	59.569	-3.698
2900	38.761	308.197	274.527	52.301	-3.607
3000	38.815	309.512	275.672	45.164	-3.523
3100	38.870	310.786	276.784	38.158	-3.444
3200	38.923	312.021	277.866	31.281	-3.370
3300	38.977	313.219	278.919	24.529	-3.300
3400	39.030	314.383	279.945	17.890	-3.235
3500	39.082	315.516	280.945	11.463	-3.174
3600	39.135	316.617	281.921	5.147	-3.116
3700	39.187	317.690	282.873	-0.959	-3.061
3800	39.239	318.736	283.803	-7.094	-3.009
3900	39.290	319.756	284.712	-13.157	-2.960
4000	39.342	320.751	285.601	-19.140	-2.913
4100	39.393	321.723	286.470	-25.043	-2.869
4200	39.444	322.673	287.321	-30.866	-2.826
4300	39.496	323.602	288.154	-36.610	-2.786
4400	39.546	324.511	288.970	-42.275	-2.748
4500	39.597	325.400	289.769	-47.862	-2.712
4600	39.648	326.271	290.553	-53.372	-2.677
4700	39.699	327.124	291.323	-58.807	-2.644
4800	39.749	327.960	292.077	-64.168	-2.612
4900	39.800	328.780	292.818	-69.455	-2.581
5000	39.850	329.585	293.545	-74.669	-2.552
5100	39.901	330.375	294.260	-79.810	-2.525
5200	39.951	331.150	294.962	-84.878	-2.498
5300	40.001	331.911	295.652	-89.875	-2.473
5400	40.051	332.659	296.330	-94.801	-2.448
5500	40.101	333.395	296.997	-99.657	-2.425
5600	40.152	334.118	297.654	-104.444	-2.402
5700	40.202	334.829	298.300	-109.163	-2.381
5800	40.252	335.529	298.936	-113.814	-2.360
5900	40.302	336.217	299.562	-118.397	-2.341
6000	40.351	336.895	300.178	-122.912	-2.322

PREVIOUS: March 1964 (1 atm)

CURRENT: March 1964 (1 bar)

Magnesium Nitride (MgN)

Mg₂N₃(g)

Mg₃O₄(cr)

Magnesium Oxide (MgO)

M_r = 40.3044

CRYSTAL

Magnesium Oxide (MgO)

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^a	S° - [G° - H°(T _r)]/T	H° - H°(T _r)	ΔG°	
0	0	INFINITE	-5.159	-597.060	INFINITE
100	7.802	52.212	-4.962	-598.962	307.976
200	26.681	14.096	-3.188	-600.646	151.347
298.15	37.106	26.924	0	-601.241	99.677
300	37.244	26.925	0.069	-601.245	99.077
400	42.561	28.460	4.087	-601.268	97.854
500	45.344	48.523	8.505	-601.046	97.153
600	47.430	57.006	13.160	-600.738	46.690
700	48.748	64.420	17.972	-600.426	39.221
800	49.740	70.996	22.878	-600.156	33.621
900	50.539	76.902	27.913	-599.962	29.268
1000	51.208	82.262	33.001	-599.826	25.749
1100	51.794	87.171	38.151	-598.406	481.399
1200	52.325	91.701	43.358	-596.495	20.560
1300	52.810	95.998	48.615	-594.101	18.414
1400	53.262	99.839	53.918	-591.324	16.550
1500	53.693	103.528	59.266	-588.172	14.722
1600	54.107	107.007	66.596	-582.877	13.125
1700	54.509	110.299	74.927	-575.371	11.719
1800	54.898	113.426	84.262	-565.653	10.472
1900	55.278	116.404	94.603	-553.777	9.358
2000	55.651	119.249	105.942	-539.749	8.358
2100	56.019	121.973	118.279	-523.579	7.455
2200	56.379	124.587	131.612	-505.271	6.636
2300	56.738	127.101	145.945	-484.824	5.890
2400	57.094	129.524	161.278	-462.249	5.208
2500	57.445	131.862	177.611	-437.543	4.582
2600	57.797	134.121	194.944	-410.707	4.005
2700	58.145	136.309	213.277	-381.741	3.473
2800	58.491	138.430	232.610	-350.755	2.979
2900	58.836	140.489	252.943	-317.749	2.521
3000	59.177	142.489	274.276	-282.723	2.095
3100	59.516	144.436	296.609	-245.677	1.697
3105.000	59.523	144.532	298.150	-244.532	1.697
3200	59.859	146.331	321.942	-205.480	1.325
3300	60.201	148.178	347.275	-163.524	0.976
3400	60.541	149.980	374.150	-118.566	0.649
3500	60.878	151.740	402.567	-70.603	0.341
3600	61.214	153.460	432.512	-19.637	0.051
3700	61.551	155.142	464.000	15.763	-0.223
3800	61.888	156.787	497.033	64.467	-0.481
3900	62.225	158.399	531.616	120.542	-0.725
4000	62.561	159.979	567.748	178.277	-0.957

$S^{\circ}(298.15 \text{ K}) = 26.924 \pm 0.08 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $T_{\text{fus}} = 3105 \pm 30 \text{ K}$

Enthalpy of Formation
 ΔH_f° is based on oxygen bomb calorimetry of Holley and Huber¹ and HCl-solution calorimetry of Shomate and Huffman.² The reported values of -143.70 ± 0.12^1 and $-143.84 \pm 0.05^2 \text{ kcal}\cdot\text{mol}^{-1}$ become $\Delta H_f^{\circ}(298.15 \text{ K}) = -143.61 \pm 0.12$ and $-143.78 \pm 0.08 \text{ kcal}\cdot\text{mol}^{-1}$ when adjusted to 1969 atomic weights. We adopt the median value of $-143.70 \pm 0.15 \text{ kcal}\cdot\text{mol}^{-1}$.
 NBS³ adopted $-143.81 \text{ kcal}\cdot\text{mol}^{-1}$ for macrocrystalline periclase, based on the data of Shomate and Huffman² converted to 1961 atomic weights. Parker⁴ preferred the data of Shomate and Huffman because of the inference that their sample corresponded more closely to the macrocrystalline standard state. New $\Delta_{\text{dis}}H_f^{\circ}$ data⁵ suggest that excess energy of up to $\sim 1.1 \text{ kcal}\cdot\text{mol}^{-1}$ arises mainly from disorder (defects) in MgO rather than from high surface area and small particle size. Since the excess energy is eliminated at $T \sim 1000^{\circ}\text{C}$,⁶ it is unlikely that this effect would bias the combustion data of Holley and Huber.
 Other data for ΔH_f° were reviewed by Parker.³ New measurements exist for $\Delta_{\text{dis}}H_f^{\circ}$ of MgO⁷ and Mg,⁸ but we have not attempted to derive ΔH_f° because of difference in the final states of the solutions.

Heat Capacity and Entropy
 C_p° below 270 K is based on data (3–270 K) for single crystals measured by Barron *et al.*⁶ Values above 270 K are from a constrained fit of C_p° and enthalpies (373–1173 K) of fused MgO measured in a Bunsen ice calorimeter by Victor & Douglas.⁷ $S^{\circ}(298.15 \text{ K})$ is obtained from C_p° based on a negligible extrapolation to absolute zero.
 Maximum deviations of the C_p° data⁶ from the adopted curve are $\pm 1.7\%$ near 15 K, $\pm 1.0\%$ near 20 K, $\pm 0.4\%$ near 40 K, and $\sim 0.2\%$ at higher temperatures. Gmelin¹⁰ later reported smoothed C_p° values (2–320 K) derived from data for MgO sintered at high temperature. These values are in good agreement with the adopted curve except from 70 to 140 K, where deviations are all positive and reach a maximum of almost 7% at 90 K. Gmelin's values gave $S^{\circ}(298.15 \text{ K}) = 6.50$, i.e., higher by $\sim 0.06 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$. Larger positive deviations in C_p° exist at all temperatures (20–301 K) for the non standard state MgO used by Giaque and Archibald.⁹ Their sample was prepared from hydroxide in vacuo at $\sim 350^{\circ}\text{C}$ and was not annealed at high temperature. The microcrystalline product presumably was disordered, leading to excess C_p° and $S^{\circ}(298.15 \text{ K}) = 6.66 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$. Limited data of Parks and Kelley¹⁰ for fused MgO tend to confirm the adopted curve.
 Deviations of the enthalpy data from the adopted curve are $\pm 0.15\%$ (373–1173 K),⁷ $-0.3 \pm 0.3\%$ (402–1799 K),¹¹ $+0.8 \pm 0.9\%$ (370–1591 K),¹² and -2.8 to $+1.0\%$ (equation for 1200–2500 K).¹³ Microcalorimetric C_p° data (305–455 K)¹⁴ agree with the adopted curve at the mid temperature but have a temperature derivative which is too small.

Fusion Data
 Refer to the liquid table for details.

- References**
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CURRENT December 1974

PREVIOUS December 1965

Mg₃O₄(cr)

Magnesium Oxide (MgO)

Mg₂O₃(l)

Magnesium Oxide (MgO)

M_r = 40.3044

LIQUID

Magnesium Oxide (MgO)

T/K	C _p ^o	S ^o	H ^o - H ^o (T _{ref})/T	H ^o - H ^o (T)	Δ _{tr} H ^o	Δ _{tr} G ^o	log K _r
0							
100							
200							
298.15	37.106	48.366	48.366	0.	-532.609	-506.707	88.773
300	37.1244	48.396	48.367	0.069	-532.614	-506.546	88.197
400	42.561	60.120	49.902	4.087	-532.636	-497.843	65.012
500	45.544	69.966	52.956	8.505	-532.414	-489.167	51.103
600	47.430	78.448	56.514	13.160	-532.106	-480.546	41.835
700	48.748	85.862	60.188	17.972	-531.794	-471.978	35.219
800	49.740	92.439	63.816	22.898	-531.525	-463.452	30.260
900	50.539	98.344	67.330	27.913	-531.331	-454.955	26.405
1000	51.208	103.705	70.704	33.001	-531.830	-445.763	23.284
1100	51.704	108.613	73.930	38.151	-530.865	-436.354	20.721
1200	52.135	113.143	77.012	43.358	-529.864	-426.943	18.584
1300	52.510	117.351	79.955	48.610	-528.829	-417.535	16.777
1400	52.862	121.281	82.768	53.918	-527.762	-408.162	15.109
1500	53.193	124.970	85.459	59.266	-526.674	-398.828	13.452
1600	54.107	128.449	88.039	64.656	-525.546	-389.540	12.004
1700	54.509	131.741	90.513	70.087	-524.370	-380.214	10.730
1800	54.898	134.868	92.891	75.538	-523.156	-370.816	9.600
1900	55.278	137.846	95.180	81.067	-521.903	-361.350	8.591
2000	55.651	140.691	97.385	86.613	-520.619	-351.874	7.686
2100	56.019	143.415	99.512	92.197	-519.304	-342.374	6.868
2100.001	56.019	143.415	99.512	92.197	GLASS → LIQUID		
2100.001	66.944	143.415	99.512	92.197	TRANSITION		
2200	66.944	146.530	101.579	98.891	-653.736	-238.077	6.128
2300	66.944	149.505	103.599	105.283	-651.037	-240.153	5.454
2400	66.944	152.354	105.571	112.280	-648.350	-222.346	4.839
2500	66.944	155.087	107.498	118.974	-645.674	-204.651	4.276
2600	66.944	157.713	109.379	125.669	-643.012	-187.062	3.781
2700	66.944	160.239	111.216	132.363	-640.362	-169.576	3.281
2800	66.944	162.674	113.011	139.057	-637.725	-152.188	2.839
2900	66.944	165.023	114.764	145.752	-635.103	-134.894	2.430
3000	66.944	167.293	116.477	152.446	-632.496	-117.690	2.049
3100	66.944	169.488	118.152	159.140	-629.904	-100.572	1.695
3105.000	66.944	169.595	118.235	159.475	CRYSTAL → LIQUID		
3200	66.944	171.613	119.790	165.835	-627.329	-83.538	1.364
3300	66.944	173.671	121.391	172.529	-624.772	-66.584	1.054
3400	66.944	175.671	122.959	179.224	-622.235	-49.708	0.764
3500	66.944	177.612	124.493	185.918	-619.719	-32.905	0.491
3600	66.944	179.498	125.994	192.612	-617.266	-16.174	0.235
3700	66.944	181.332	127.465	199.307	-614.877	0.467	-0.007
3800	66.944	183.117	128.806	206.001	-612.515	17.083	-0.235
3900	66.944	184.856	130.119	212.696	-610.180	33.615	-0.450
4000	66.944	186.551	131.704	219.390	-607.784	50.084	-0.647
4100	66.944	188.204	133.062	226.084	-605.367	66.495	-0.847
4200	66.944	189.817	134.394	232.779	-602.851	82.849	-1.030
4300	66.944	191.393	135.701	239.473	-600.272	99.149	-1.204
4400	66.944	192.932	136.984	246.168	-597.638	115.395	-1.370
4500	66.944	194.436	138.244	252.862	-594.953	131.591	-1.527
4600	66.944	195.907	139.482	259.556	-592.217	147.739	-1.678
4700	66.944	197.347	140.698	266.251	-589.430	163.840	-1.821
4800	66.944	198.756	141.893	272.945	-586.597	179.897	-1.958
4900	66.944	200.137	143.067	279.640	-583.796	195.912	-2.088
5000	66.944	201.489	144.222	286.334	-581.028	211.886	-2.214

Enthalpy Reference Temperature = T_r = 298.15 K
 S^o(298.15 K) = [48.366] J·K⁻¹·mol⁻¹
 T_{ref} = 3105 ± 30 K
 Δ_{tr}H^o(298.15 K) = [-532.609] kJ·mol⁻¹
 Δ_{tr}H^o = [77.822 ± 16.7] kJ·mol⁻¹
 Enthalpy of Formation
 Δ_fH^o(MgO, l, 298.15 K) is calculated from that of the crystal by adding Δ_{tr}H^o and the difference in enthalpy, H^o(3105 K) - H^o(298.15 K).
 to between the crystal and liquid.

Heat Capacity and Entropy
 C_p^o is assumed to be 16 cal·K⁻¹·mol⁻¹ except below the glass transition (2100 K) where C_p^o (cr) is taken equal to C_p^o (l). Enthalpy data yield C_p^o ≥ 19 cal·K⁻¹·mol⁻¹ for liquid BeO¹ but there may be a positive bias due to volatilization. S^o(298.15 K) is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data
 Documented values for T_{fus} (in °C, IPTS-48) include 2800 ± 20,² 2827 ± 20³ and 2852.^{4,5} We adopt the median value³ which becomes 2832°C = 3105 K on IPTS-68.
 Calorimetric data for Δ_{tr}H^o are not available. Kelley⁶ derived an apparent Δ_{tr}H^o = 18.5 kcal·mol⁻¹ at T_{fus} = 2915 K from liquidus data for the MgO-ZrO₂ binary. The old⁷ and new^{8,9} data for MgO-ZrO₂ imply gross non-ideality which makes the system unsuitable for obtaining the enthalpy of fusion. Apparent Δ_{tr}H^o values ranging from 8 to 30 kcal·mol⁻¹ are obtained from more suitable binary systems^{9,10} involving CaO, Al₂O₃, Cr₂O₃, PuO₂, and UO₂. These values are so uncertain that we assume Δ_{tr}H^o = 18.6 kcal·mol⁻¹ based on Δ_{tr}H^o = 6 cal·K⁻¹·mol⁻¹. Δ_{tr}H^o = 20 kcal·mol⁻¹ was measured calorimetrically for BeO¹, but the crystal is hexagonal or tetragonal rather than cubic as in the case of MgO.

Vaporization Data
 Vaporization rates based on weight loss at T_{ref} were reported by Noguchi⁸ for MgO and six other refractory oxides. Vaporization of MgO near 2000 K has been studied by Langmuir-torsion,¹¹ Langmuir-weight-loss,^{12,13} Knudsen-mass-spectrometric,¹⁴ Knudsen-effusion¹⁵ and transpiration¹⁶ methods. Vaporization near 2000 K is primarily to the elements,¹⁴ Mg(g) and presumably O(g) and O₂(g), rather than to MgO(g). Quantitative interpretation of the vaporization species is uncertain. The adopted tables¹ predict that MgO(g) is insignificant near 2000 K but should become one of the significant components of the vapor near T_{ref}.

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PREVIOUS: December 1965

CURRENT: December 1974

Mg₂O₃(l)

Magnesium Oxide (MgO)

Magnesium Oxide (MgO)

M_r = 40.3044 Magnesium Oxide (MgO)Mg₁O₁(cr,l)

0 to 3105 K crystal
above 3105 K liquid

Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^o	S° - [G° - H°(T _r)]/T	H° - H°(T _r)	Δ _r H°	
J·K ⁻¹ ·mol ⁻¹					
0	0	0	INFINITE	-579.060	INFINITE
100	7.802	2.548	52.212	-4.966	307.976
200	26.681	14.096	30.037	-3.188	151.347
298.15	37.106	26.924	26.924	0	99.677
300	37.244	26.925	26.925	0.069	99.077
400	42.561	38.678	28.460	4.087	72.854
500	45.544	48.523	31.513	8.505	57.153
600	47.430	57.006	35.072	13.160	46.690
700	48.748	64.420	38.746	17.972	39.221
800	49.740	70.996	42.374	22.898	33.621
900	50.539	76.902	45.888	27.913	29.268
1000	51.208	82.262	49.262	33.001	25.749
1100	51.794	87.171	52.488	38.151	22.860
1200	52.325	91.701	55.569	43.358	20.452
1300	52.810	95.908	58.512	48.615	18.414
1400	53.262	99.839	61.325	53.918	16.550
1500	53.693	103.528	64.017	59.266	14.722
1600	54.107	107.007	66.596	64.656	13.125
1700	54.509	110.299	69.071	70.087	11.719
1800	54.898	113.446	71.449	75.558	10.481
1900	55.278	116.464	73.717	81.067	9.352
2000	55.651	119.249	75.942	86.613	8.358
2100	56.019	121.973	78.070	92.197	7.455
2200	56.379	124.587	80.125	97.816	6.636
2300	56.738	127.101	82.114	103.472	5.890
2400	57.094	129.524	84.039	109.164	5.208
2500	57.445	131.862	85.905	114.891	4.582
2600	57.797	134.121	87.716	120.659	4.005
2700	58.145	136.309	89.476	126.450	3.473
2800	58.491	138.430	91.187	132.282	2.979
2900	58.836	140.489	92.851	138.148	2.521
3000	59.177	142.489	94.473	144.049	2.095
3100	59.516	144.436	96.053	149.987	1.697
3105.000	59.523	144.532	96.131	150.284	1.697
3105.000	66.944	169.595	96.131	228.107	CRYSTAL <- -> LIQUID TRANSITION
3200	66.944	171.613	98.342	234.466	-83.538
3300	66.944	173.673	100.594	241.161	-66.584
3400	66.944	175.671	102.773	247.855	-49.708
3500	66.944	177.612	104.884	254.550	-32.905
3600	66.944	179.498	106.930	261.244	-16.174
3700	66.944	181.332	108.916	267.938	0.487
3800	66.944	183.117	110.846	274.633	17.083
3900	66.944	184.856	112.721	281.327	33.615
4000	66.944	186.551	114.546	288.022	50.084
4100	66.944	188.204	116.322	294.716	66.495
4200	66.944	189.817	118.053	301.410	82.849
4300	66.944	191.393	119.740	308.105	99.149
4400	66.944	192.932	121.386	314.799	115.395
4500	66.944	194.436	122.993	321.494	131.591
4600	66.944	195.907	124.562	328.188	147.739
4700	66.944	197.347	126.095	334.882	163.840
4800	66.944	198.756	127.595	341.577	179.897
4900	66.944	200.137	129.061	348.271	195.912
5000	66.944	201.489	130.496	354.966	211.886

PREVIOUS:

CURRENT: December 1974

Magnesium Oxide (MgO)

Mg₁O₁(cr,l)

Mg₁O₁(g)

MgO

IDEAL GAS

Magnesium Oxide (MgO)

Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$

Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$

Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$

T/K	C_p°	S°	$-(G^\circ - H^\circ(T))/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\log K_r$
0	0	0	0	0	0	INFINITE
100	29.124	180.485	240.493	-8.909	58.588	INFINITE
200	30.117	206.173	216.143	-6.001	59.402	-26.624
250	31.121	207.699	213.793	-3.054	58.886	-11.149
298.15	32.173	213.269	213.269	0	58.517	-8.082
300	32.175	213.269	213.270	0.060	58.144	-6.113
350	33.401	218.522	213.666	1.699	30.880	-3.609
400	34.783	223.069	214.562	3.403	30.860	-3.534
450	36.452	227.259	215.743	5.182	23.280	-2.702
500	38.434	231.200	217.093	7.053	17.451	-2.040
600	43.078	238.608	220.068	11.174	12.088	-1.052
700	47.785	245.608	223.271	15.671	6.666	-0.348
800	51.460	252.250	226.139	20.649	2.783	0.182
900	53.890	258.472	228.657	25.934	0.577	0.597
1000	54.795	264.208	232.829	31.379	49.315	0.894
1100	54.608	269.429	235.923	36.837	49.607	1.129
1200	53.729	274.147	238.915	42.278	49.823	1.326
1300	52.496	278.400	241.792	47.914	49.914	1.493
1400	51.139	282.241	244.546	52.731	49.885	1.518
1500	49.802	285.723	247.177	57.820	49.693	1.327
1600	48.558	288.897	249.687	62.737	49.399	1.161
1700	47.439	291.807	252.080	67.535	48.925	1.017
1800	46.454	294.490	254.363	72.229	48.379	0.891
1900	45.599	296.978	256.541	76.831	47.768	0.779
2000	44.862	299.298	258.621	81.353	47.092	0.679
2100	44.230	301.471	260.611	85.806	46.364	0.589
2200	43.691	303.516	262.515	90.202	45.598	0.507
2300	43.231	305.447	264.340	94.547	44.799	0.434
2400	42.841	307.279	266.091	98.850	43.977	0.366
2500	42.509	309.021	267.774	103.117	43.131	0.305
2600	42.229	310.682	269.392	107.354	42.269	0.248
2700	41.993	312.272	270.951	111.565	41.399	0.195
2800	41.795	313.795	272.462	115.754	40.522	0.147
2900	41.629	315.259	273.905	119.923	40.163	0.102
3000	41.493	316.668	275.300	124.081	39.804	0.059
3100	41.381	318.026	276.664	128.224	39.453	0.020
3200	41.291	319.339	277.977	132.357	39.109	0.017
3300	41.220	320.608	279.250	136.483	38.772	0.051
3400	41.167	321.838	280.484	140.602	38.442	0.084
3500	41.128	323.030	281.683	144.717	38.124	0.115
3600	41.103	324.189	282.848	148.828	37.824	0.144
3700	41.091	325.315	283.980	152.938	37.539	0.172
3800	41.090	326.411	285.082	157.047	37.267	0.198
3900	41.099	327.478	286.156	161.156	37.007	0.223
4000	41.117	328.519	287.202	165.267	36.764	0.246
4100	41.144	329.534	288.222	169.380	36.537	0.269
4200	41.179	330.526	289.218	173.496	36.326	0.290
4300	41.222	331.496	290.190	177.616	36.131	0.311
4400	41.272	332.444	291.139	181.741	35.952	0.331
4500	41.329	333.372	292.075	185.871	35.790	0.350
4600	41.393	334.281	292.975	190.007	35.643	0.368
4700	41.463	335.172	293.849	194.149	35.510	0.386
4800	41.539	336.046	294.733	198.300	35.389	0.403
4900	41.621	336.903	295.585	202.458	35.279	0.419
5000	41.709	337.745	296.420	206.624	35.179	0.435
5100	41.802	338.572	297.238	210.800	35.089	0.451
5200	41.901	339.384	298.041	215.083	35.007	0.466
5300	42.004	340.183	298.829	219.466	34.933	0.480
5400	42.113	340.970	299.602	223.866	34.866	0.494
5500	42.227	341.743	300.361	228.266	34.805	0.508
5600	42.345	342.505	301.107	232.666	34.749	0.521
5700	42.467	343.256	301.840	237.066	34.697	0.534
5800	42.594	343.995	302.561	241.466	34.649	0.547
5900	42.725	344.725	303.269	245.866	34.605	0.559
6000	42.860	345.444	303.966	250.266	34.565	0.572

$\Delta_f H^\circ(0 \text{ K}) = -58.59 \pm 25.1 \text{ kJ mol}^{-1}$
 $\Delta_f H^\circ(298.15 \text{ K}) = -58.16 \pm 25.1 \text{ kJ mol}^{-1}$

$S^\circ(298.15 \text{ K}) = 213.269 \pm 3.3 \text{ J K}^{-1} \text{ mol}^{-1}$

State	ϵ_r , cm ⁻¹	ω_e , cm ⁻¹	$\omega_e x_e$, cm ⁻¹	B_e , cm ⁻¹	α_e , cm ⁻¹	r_e , Å	Source
X ¹ Σ ⁺	0.0	785.1	5.18	0.5743	[0.0050]	1.749	1
X ³ Π	[2300]	[664.4]	[3.9]	[0.5050]	[0.0040]	[1.864]	2-7
A ¹ Π	3503.3	664.4	3.9	0.5050	0.0040	1.864	1
B ³ Σ ⁻	[14000]	[824.1]	[4.8]	[0.5822]	[0.0045]	[1.737]	2-5
B ¹ Σ ⁺	20004.	824.1	4.76	0.5822	0.0045	1.737	4,3
Z ³ Σ ⁻	[28000]	[632.5]	[5.3]	[0.5011]	[0.0048]	[1.872]	4,3
Z ¹ Σ ⁺	[29000]	[632.5]	[5.3]	[0.5011]	[0.0048]	[1.872]	4,3
D ¹ Δ	29775.	632.5	5.3	0.5014	0.0048	1.872	1,1,9
Z ³ Σ ⁻	[30000]	[632.5]	[5.3]	[0.5011]	[0.0048]	[1.872]	4,3
C ¹ Σ ⁺ *	30004.	632.4	5.2	0.5008	0.0048	1.873	1,1,4
E ¹ Σ ⁺	37684.	[632.4]	[5.2]	0.5273	[0.0048]	1.825	4,3
F ³ Π	[37000]	[710]	[5.1]	[0.5615]	[0.005]	[1.768]	10,4
F ¹ Π	37879.	710	[5.1]	[0.5615]	[0.005]	1.768	4,3
G ³ Π	[39000]	[790]	[5.1]	[0.5249]	[0.005]	[1.83]	10,4
G ¹ Π	39868.	790	[5.1]	0.5249	[0.005]	1.83	10,4

Enthalpy of Formation
 We adopt $D_0^\circ = 80 \pm 6 \text{ kcal mol}^{-1}$ and $\Delta_f H^\circ(298.15 \text{ K}) = 13.9 \pm 6 \text{ kcal mol}^{-1}$ based on equilibria analyzed below. Greatest weight is given to mass-spectrometric data¹¹ for reactions A and B. We give ω_e , $\omega_e x_e$, or ν_e for $\Delta_f H^\circ$ and D_0° values which may have a systematic bias. The JANAF differences in $\Delta_f H^\circ(298.15 \text{ K})$ for WO_3 and WO_2 may be biased by as much as $-3.5 \text{ kcal mol}^{-1}$, leading to a positive bias in D_0° from reaction B. Mass spectra¹² and transpiration data¹³ yield an upper limit to D_0° ; we neglect $\text{Mg}(\text{OH})_2$ and MgOH which probably are important in.¹³ Cotton and Jenkins¹⁴ concluded that hydroxides were negligible in their H_2 - O_2 - N_2 flames; we doubt this conclusion and presume that reaction D yields an upper limit to D_0° . Our adopted value is comparable with those of Richards *et al.*¹⁵ and Brewer & Rosenblatt,¹⁶ considering the difference in functions for MgO.

Other published values of D_0° are dismissed for reasons cited in critical reviews.^{17,18,11} Schofield's criticism¹⁷ of flame studies is supported by new evidence for importance of hydroxides (CaO , g).¹⁸ Inadequate allowance for hydroxides may bias a recent flame result of $D_0^\circ = 88 \pm 2.3 \text{ kcal mol}^{-1}$,¹⁹ furthermore, we cannot firm this D_0° from the published information. $D_0^\circ = 83 \text{ kcal mol}^{-1}$ was derived²⁰ by fitting an electron-impact potential function to X¹Σ. This state is predicted^{16,41} to dissociate to excited state O¹D at 45.4 kcal mol⁻¹. Theoretical calculations¹⁶ support this prediction. Linear Birge-Sponner extrapolation yields a very low estimate for D_0° , just as it does for the alkali halides,¹⁸ unless X¹Σ fails to dissociate to O¹D as predicted.

Source	Method	Reaction ^a	T/K	ΔS	Data Points	$\Delta_f H^\circ(298.15 \text{ K})$, kcal mol ⁻¹	D_0° , kcal mol ⁻¹		
11	Knudsen mass spec.	A	2026-2274	8	-13 ± 5	12 ± 11	39.5 ± 3	15.3	78.6 ± 3
	Knudsen mass spec.	B	2106-2225	6	-18 ± 8	23 ± 16	63.1 ± 3	>10.1	<83.8 ± 5
12	Knudsen mass spec.	C	1950	1	—	—	>148.7	>5.0	<86.9 ± 5
13	Transpiration	C	1780-2010	7	-8 ± 3	132 ± 5	>148.3 ± 2	>4.7	<89.2 ± 2
14	Transpiration	C	2033-2175	8	-52 ± 32	53 ± 68	162.8 ± 8	19.1	74.7 ± 8
15	Flame spec.	D	1570-2370	4	-9 ± 1	-11 ± 2	>5.7 ± 6	>-1.6	<95.4 ± 6

^aReactions: A) $\text{Mg}(\text{g}) + \text{O}(\text{g}) = \text{MgO}(\text{g}) + \text{O}(\text{g})$
 B) $\text{Mg}(\text{g}) + \text{WO}_3(\text{g}) = \text{MgO}(\text{g}) + \text{WO}_2(\text{g})$
 C) $\text{MgO}(\text{cr}) = \text{MgO}(\text{g})$
 D) $\text{Mg}(\text{g}) + \text{OH}(\text{g}) = \text{MgO}(\text{g}) + \text{H}(\text{g})$

Heat Capacity and Entropy
 Electronic levels (T_0) and vibrational-rotational constants of observed states are from Rosen¹ and other recent sources.¹⁻¹⁰ States are listed in the isoelectronic order given by Schamps and Lefebvre-Brion.⁴ Designations² of the new E, F and G states are based on theoretical calculations.⁴ Field² concluded that calculations⁴⁻⁶ of the isoelectronic A¹Π-Π separation should be adequate for estimating the low-lying Π state. The other potentially low-lying state (Σ⁺) is estimated⁴ similarly from isoelectronic B³Σ⁻. Higher estimated levels are also based on calculations.⁴ Vibrational-rotational constants are estimated in isoelectronic groups by comparison with BeO, CaO, SrO and BaO.³ Low-lying levels and their vibrational-rotational constants cause marked changes in the thermodynamic functions, which are calculated using first-order anharmonic corrections to Q_r and Q_v ; in the partition function $Q = Q_r Q_v Q_e \exp(-c_v/T)$.

Mg₁O₁(g)

Magnesium Oxide (MgO)

IDEAL GAS

Magnesium Oxide (MgO)

Mg₁₀O₃Si₁(cr)

Magnesium Silicate (MgSiO₃)

$M_r = 100.3887$

CRYSTAL(I-II-III)

Magnesium Silicate (MgSiO₃)

T/K	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^o	S° - [G° - H°(T)]/T	H° - H°(T)	ΔG°	
0	0	0	INFINITE	-1539.788	INFINITE
100	23.912	11.117	124.420	-1518.053	792.950
200	59.643	39.430	74.617	-1547.531	389.255
298.15	81.927	67.768	67.768	-1548.917	256.140
300	82.278	68.278	67.760	-1548.930	254.467
400	94.194	93.738	71.160	-1549.184	187.050
500	101.512	115.590	77.915	-1548.910	146.578
600	106.900	134.600	85.812	-1548.358	119.613
700	111.621	151.449	94.008	-1547.624	100.361
800	115.780	166.629	102.152	-1546.754	85.979
900	119.675	180.492	110.097	-1545.768	74.711
903.000	119.788	180.891	110.332	-1545.768	74.711
903.000	120.340	181.652	110.332	-1552.726	65.709
1000	120.340	193.911	117.854	-1552.726	65.709
1100	120.340	205.381	125.298	-1552.043	58.337
1200	120.340	215.852	132.414	-1551.461	52.197
1258.000	120.340	221.552	136.393	-1551.461	52.197
1258.000	122.432	222.829	136.393	-1549.254	47.005
1300	122.432	226.850	139.250	-1549.254	47.005
1400	122.432	235.923	145.836	-1549.254	47.005
1500	122.432	244.370	152.126	-1549.254	47.005
1600	122.432	252.271	158.141	-1549.254	47.005
1700	122.432	259.694	163.859	-1549.254	47.005
1800	122.432	266.692	169.417	-1549.254	47.005
1850.000	122.432	270.046	172.091	-1549.254	47.005
1900	122.432	273.311	174.712	-1549.254	47.005
2000	122.432	279.591	179.801	-1549.254	47.005
2100	122.432	285.565	184.696	-1549.254	47.005
2200	122.432	291.260	189.411	-1549.254	47.005
2300	122.432	296.703	193.959	-1549.254	47.005
2400	122.432	301.913	198.349	-1549.254	47.005
2500	122.432	306.911	202.592	-1549.254	47.005

$S^{\circ}(298.15 \text{ K}) = 67.77 \pm 0.8 \text{ J K}^{-1} \text{ mol}^{-1}$
 $T_{\text{m1}} = 903 \text{ K} = 0.67 \text{ kJ mol}^{-1}$
 $T_{\text{m2}} = 1258 \text{ K}$
 $T_{\text{m3}} = 1850 \pm 2 \text{ K}$

Enthalpy of Formation
 Torgeson *et al.*¹ report a $\Delta_f H^{\circ}(298.15 \text{ K}) = -8.69 \pm 0.15 \text{ kcal mol}^{-1}$ for reaction (a). They used a hydrofluoric acid solution calorimeter and measured the enthalpies of solution of each component. They appear to have made the water-absorption correction to the enthalpy of solution of SiO₂(cr) in the wrong direction. We reverse the correction so that the new $\Delta_f H^{\circ}$ almost overlaps the range observed by King.¹¹ We derive $\Delta_f H^{\circ}(\text{MgSiO}_3, \text{cr}, 298.15 \text{ K}) = -370.20 \pm 1.0 \text{ kcal mol}^{-1}$ using the $\Delta_f H^{\circ}(298.15 \text{ K})$ of MgO(cr) and SiO₂(cr, low quartz) from the JANAF tables.
 Reesman *et al.*² calculated a $\Delta_f G^{\circ}(298.15 \text{ K}) = 23.72 \text{ kcal mol}^{-1}$ for reaction (b) using aqueous solubility data. We use the $\Delta_f G^{\circ}(298.15 \text{ K})$ of H₂O(l) and OH⁻(aq) from source 3, $\Delta_f G^{\circ}(298.15 \text{ K})$ of H₂SiO₄(aq) from source 4 and $\Delta_f G^{\circ}(298.15 \text{ K})$ of Mg²⁺(aq) from source 5 and we obtain a $\Delta_f G^{\circ}(\text{MgSiO}_3, \text{cr}, 298.15 \text{ K}) = -352.534 \text{ kcal mol}^{-1}$. We derive $\Delta_f H^{\circ}(\text{MgSiO}_3, \text{cr}, 298.15 \text{ K}) = -373.293 \text{ kcal mol}^{-1}$ using the above $\Delta_f G^{\circ}(298.15 \text{ K})$ of MgSiO₃(cr) and the entropies of Mg(cr), Si(cr) and O₂(g) from the JANAF tables.
 We choose the enthalpy of formation derived from the result of Torgeson *et al.*¹ which is considered to be better since it relates directly to the oxides. Also the $\Delta_f G^{\circ}(\text{MgSiO}_3, \text{cr}, 1873 \text{ K})$ thus calculated is in very good agreement with that derived from the activities of SiO₂ and MgO (in the SiO₂-MgO system) measured by Rein *et al.*⁶ The $\Delta_f H^{\circ}(\text{MgSiO}_3, \text{cr}, 298.15 \text{ K})$ derived from the work of Reesman *et al.*² is less accurate and involves uncertainties in the auxiliary data used to calculate the value.

Source	Method	Reaction	$\Delta_f H^{\circ}(298.15 \text{ K})$ kcal mol ⁻¹	$\Delta_f G^{\circ}(298.15 \text{ K})$ kcal mol ⁻¹	$\Delta_f H^{\circ}(298.15 \text{ K})$ kcal mol ⁻¹
1	HF solution calorimeter	(a) MgO(cr) + SiO ₂ (cr) = MgSiO ₃ (cr)	-8.7 ± 0.15	23.72	-370.20
2	Aqueous solubility	(b) MgSiO ₃ (cr) + 3H ₂ O(l) = Mg ²⁺ (aq) + H ₄ SiO ₄ (aq) + 2OH ⁻ (aq)	-8.7 ± 0.15	23.72	-373.3

Heat Capacity and Entropy
 Low temperature heat capacities are from the data (53–295 K) of Kelley.⁷ Wagner⁸ measured the average heat capacities in the temperature range 580–1570 K. Using his data we derive the high temperature heat capacities which are joined smoothly with the low temperature values by a constrained fitting technique. The C_p^o values at 903 = 1258 K and above 1258 K are derived as 28.762 and 29.262 cal K⁻¹ mol⁻¹, respectively, by assuming that the data of Wagner⁸ pertain to the stable phase in these regions. The entropy is based on S^o(50 K) = 0.49 cal K⁻¹ mol⁻¹.

Transition Data
 $T_{\text{m1}} = 903 \text{ K}$ is obtained from Boyd *et al.*⁹ The authors determined the phase diagram boundary at high pressures and extrapolated to one atmosphere. $T_{\text{m2}} = 1258 \text{ K}$ is taken from Atlas.¹⁰ Below 903 K the phase is known as clinoenstatite. Between 903 and 1258 K it is rhombic enstatite and above 1258 K it is protoenstatite. We calculate $\Delta_{\text{m1}} H^{\circ}$ and $\Delta_{\text{m2}} H^{\circ}$ (from dT/dP (slopes of the inversion) = 2.6/kbar and 84/kbar reported by Boyd *et al.*⁹) and from the densities of clinoenstatite (3.210 gm/cc) and rhombic enstatite (3.208 gm/cc) reported by Stephenson *et al.*¹¹ and the density of protoenstatite (3.10 gm/cc) reported by Smith.¹²

Fusion Data
 Refer to the liquid table for details.

References
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¹²J. V. Smith, *Acta Cryst.* **12**, 515 (1959).
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Magnesium Silicate (MgSiO₃)

S°(298.15 K) = [92.515] J·K⁻¹·mol⁻¹
 T_{m1} = 903 K
 T_{m2} = 1258 K
 T_{liq} = 1850 ± 2 K

LIQUID

ΔH°(298.15 K) = [-1494.862 ± 20.9] kJ·mol⁻¹
 Δ_{cr}H° = 0.67 kJ·mol⁻¹
 Δ_{liq}H° = 1.632 kJ·mol⁻¹
 Δ_{liq}H° = [75.312 ± 20.9] kJ·mol⁻¹

M_r = 100.3887 Magnesium Silicate (MgSiO₃)

ΔH°(298.15 K) = [-1494.862 ± 20.9] kJ·mol⁻¹
 Δ_{cr}H° = 0.67 kJ·mol⁻¹
 Δ_{liq}H° = 1.632 kJ·mol⁻¹
 Δ_{liq}H° = [75.312 ± 20.9] kJ·mol⁻¹

Mg₁O₃Si₁(l)

Enthalpy Reference Temperature = T_r = 298.15 K
 Standard State Pressure = p° = 0.1 MPa
 kJ·mol⁻¹
 Δ_{cr}H°
 Δ_{liq}H°
 H° - H°(T_r)/T
 S° - S°(T_r)/T
 C_p
 T/K
 0
 100
 200
 298.15
 300
 400
 500
 600
 700
 800
 900
 900.000
 1000
 1100
 1200
 1300
 1400
 1500
 1600
 1700
 1800
 1850.000
 1900
 2000
 2100
 2200
 2300
 2400
 2500
 2600
 2700
 2800
 2900
 3000

Enthalpy of Formation

Δ_fH°(MgSiO₃, l, 298.15 K) is calculated from Δ_fH°(MgSiO₃, cr, 298.15 K) by adding Δ_{cr}H° and the difference in enthalpy. H°(1850 K) - H°(298.15 K), between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 900 K. Below 900 K the heat capacity is obtained from the heat capacity of the crystal. Above 900 K the heat capacity is assumed constant and estimated as 35 cal·K⁻¹·mol⁻¹ or 7 cal·K⁻¹·g-atom⁻¹. S°(l, 298.15 K) is calculated in a manner analogous to that used for the enthalpy of formation.

Transition Data

Refer to the crystal table for details.

Fusion Data

T_m is taken from Bowen and Andersen.¹ MgSiO₃(cr) melts incongruently in the temperature range 1830–1850 K at atmospheric pressure. Δ_{liq}H° is estimated from the phase diagrams of the MgSiO₃-TiO₂ system reported by MacGregor.² The phase diagrams were determined at 10 and 20 kbars pressure where MgSiO₃(cr) melts congruently.

References

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T/K	C _p	S°	S° - S°(T _r)/T	H° - H°(T _r)/T	Δ _{cr} H°	Δ _{liq} H°	log K _r
0							
100							
200							
298.15	81.927	92.515	0.	0.	-1494.862	-1415.346	247.963
300	82.228	93.022	92.516	0.152	-1494.875	-1414.853	246.348
400	94.194	118.484	95.906	9.031	-1495.129	-1388.130	181.270
500	101.512	140.337	102.661	18.838	-1494.855	-1361.392	142.224
600	106.997	159.347	110.559	29.273	-1494.303	-1334.747	116.200
700	111.621	176.195	118.754	40.208	-1492.569	-1308.211	97.620
800	115.780	191.375	126.899	51.581	-1492.699	-1281.789	83.620
900	119.675	205.239	134.844	63.356	-1491.713	-1255.483	72.866
900.000	119.675	205.239	134.844	63.356	GLASS <- -> LIQUID		
1000	146.440	220.668	142.668	78.000	TRANSITION		
1100	146.440	234.625	150.404	92.644	-1496.729	-1228.717	64.182
1200	146.440	247.367	157.961	107.288	-1493.435	-1202.076	57.082
1300	146.440	259.088	165.295	121.932	-1490.244	-1175.731	51.178
1400	146.440	269.941	172.387	136.576	-1487.146	-1149.648	46.193
1500	146.440	280.044	179.231	151.220	-1481.545	-1120.632	41.811
1600	146.440	289.495	185.830	165.864	-1472.265	-1085.717	37.808
1700	146.440	298.373	192.192	180.508	-1460.067	-1051.085	34.314
1800	146.440	306.743	198.326	195.152	-1449.124	-1016.266	31.226
1850.000	146.440	310.756	201.310	202.474	-1444.852	-979.163	28.415
1900	146.440	314.661	204.242	209.796	--- III <- -> LIQUID ---		
2000	146.440	322.172	209.952	224.440	-1640.616	-942.295	25.906
2100	146.440	329.317	215.468	239.084	-1636.414	-905.650	23.653
2200	146.440	336.129	220.799	253.728	-1632.247	-869.215	21.621
2300	146.440	342.639	225.956	268.372	-1628.114	-832.976	19.777
2400	146.440	348.871	230.948	283.016	-1624.015	-796.976	18.099
2500	146.440	354.849	235.786	297.660	-1619.951	-761.053	16.564
2600	146.440	360.593	240.476	312.304	-1615.921	-725.349	15.155
2700	146.440	366.120	245.028	326.948	-1611.924	-689.805	13.858
2800	146.440	371.445	249.448	341.592	-1607.962	-654.414	12.660
2900	146.440	376.584	253.744	356.236	-1604.033	-619.169	11.551
3000	146.440	381.549	257.922	370.880	-1600.138	-584.065	10.520
					-1596.278	-549.093	9.561

PREVIOUS: September 1964

CURRENT: December 1967

Magnesium Silicate (MgSiO₃)

Mg₁O₃Si₁(l)

$M_r = 100.3887$

Magnesium Silicate ($MgSiO_3$)

CRYSTAL(I-II-III)-LIQUID

Magnesium Silicate ($MgSiO_3$)

0 to 903 K crystal, I
 903 to 1258 K crystal, II
 1258 to 1850 K crystal, III
 above 1850 K liquid

Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa		$\log K_r$
	C_p°	$S^\circ - (G^\circ - H^\circ(T_r))/T_r$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	
	$J \cdot K^{-1} \cdot mol^{-1}$	$J \cdot K^{-1} \cdot mol^{-1}$	$KJ \cdot mol^{-1}$	$KJ \cdot mol^{-1}$	
0	0	0	INFINITE	INFINITE	INFINITE
100	23.912	11.117	124.420	-1539.788	-1539.788
200	59.645	39.450	74.617	-1548.271	-1548.053
298.15	81.927	67.768	67.768	-1547.531	-1490.410
300	82.228	68.276	67.770	-1548.917	-1462.023
400	94.194	93.738	71.160	0	-1461.484
500	101.512	115.590	77.915	0.152	-1431.276
600	106.997	134.600	85.812	18.838	-1403.073
700	111.621	151.449	94.008	29.273	-1373.955
800	115.780	166.629	102.152	40.208	-1344.943
900	119.675	180.492	110.097	51.581	-1316.047
903.000	119.788	180.891	110.332	63.715	-1287.267
903.000	120.340	181.632	110.332	64.384	TRANSITION
1000	120.340	193.911	117.854	76.057	-1257.958
1100	120.340	205.381	125.298	88.091	-1228.515
1200	120.340	215.852	132.414	100.125	-1199.129
1258.000	120.340	221.532	136.393	107.105	TRANSITION
1258.000	122.432	222.829	136.393	108.737	II < -> III
1300	122.432	226.850	139.250	113.879	-1169.845
1400	122.432	235.923	145.836	126.172	-1137.516
1500	122.432	244.370	152.126	138.365	-1099.115
1600	122.432	252.271	158.141	150.609	-1060.837
1700	122.432	259.694	163.899	162.852	-1022.222
1800	122.432	266.692	169.417	175.095	-981.182
1850.000	122.432	270.046	172.091	181.217	TRANSITION
1850.000	146.440	310.756	172.091	256.529	III < -> LIQUID
1900	146.440	314.661	175.792	263.851	-942.295
2000	146.440	322.172	182.925	278.495	-903.650
2100	146.440	329.317	189.727	293.139	-869.215
2200	146.440	336.129	196.228	307.783	-832.976
2300	146.440	342.639	202.453	322.427	-796.926
2400	146.440	348.871	208.425	337.071	-761.053
2500	146.440	354.849	214.164	351.715	-725.349
2600	146.440	360.593	219.686	366.359	-689.805
2700	146.440	366.120	225.007	381.003	-654.414
2800	146.440	371.445	230.143	395.647	-619.169
2900	146.440	376.584	235.104	410.291	-584.065
3000	146.440	381.549	239.904	424.935	-549.093

PREVIOUS.

CURRENT December 1967

Magnesium Silicate ($MgSiO_3$)

$Mg_1O_3Si_1(cr, l)$

Magnesium Titanium Oxide (MgTiO₃)

CRYSTAL

M_r = 120.1832 Magnesium Titanium Oxide (MgTiO₃)

Mg₁O₃Ti₁(cr)

S^o(298.15 K) = 74.56 ± 0.4 J·K⁻¹·mol⁻¹
 T_m = 1953 ± 20
 $\Delta_f H^{\circ}(0 \text{ K}) = -1563.26 \pm 6.3 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_f H^{\circ}(298.15 \text{ K}) = -1572.56 \pm 6.3 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{sub}} H^{\circ} = [90.374] \text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation

The adopted enthalpy of formation is calculated from $\Delta_f H^{\circ}(298.15 \text{ K}) = -6.35 \pm 0.25 \text{ kcal}\cdot\text{mol}^{-1}$ for the reaction MgO(cr) + TiO₂(rutile) → MgTiO₃(cr) measured by Kelley *et al.*,¹ using a solution calorimetric method. For the same reaction a value of $\Delta_f H^{\circ}(298.15 \text{ K}) = -5.5 \pm 0.1 \text{ kcal}\cdot\text{mol}^{-1}$ was obtained with a calorimetric bomb method by Ronflov and Feodos'ev.² These authors used the oxidation of lampblack in order to initiate the formation of the titanate from the oxides. Unfortunately the desired enthalpy of reaction was only 1.2 to 1.5 percent of the total measured heat, and consequently this result appears to be more uncertain than that measured by the solution calorimetric method.

Heat Capacity and Entropy

Low temperature heat capacities are from the data (52–296 K) of Shomate.³ High temperature enthalpies have been measured (402–1720 K) by Naylor and Cook.⁴ High temperature heat capacities are derived from the enthalpies by a fitting technique which constrains the curve to join smoothly with the low temperature values. The entropy is based on S^o(52 K) = 0.45 cal·K⁻¹·mol⁻¹.

Fusion Data

Refer to the liquid table for details.

References

- ¹K. K. Kelley, S. S. Todd and E. G. King, U. S. Bur. Mines RI 5059, (1954).
- ²B. I. Ronflov and N. N. Feodos'ev, Russ. J. Inorg. Chem. 9, 1452 (1964).
- ³C. H. Shomate, J. Amer. Chem. Soc. 67, 964 (1946).
- ⁴B. F. Naylor and O. A. Cook, J. Amer. Chem. Soc. 68, 1003 (1946).

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = P ^o = 0.1 MPa	
	S ^o	-(G ^o - H ^o (T _r))/T	H ^o - H ^o (T _r)	Δ _f G ^o
	J·K ⁻¹ ·mol ⁻¹	J·K ⁻¹ ·mol ⁻¹	kJ·mol ⁻¹	kJ·mol ⁻¹
0	0.	INFINITE	-13.556	-1563.260
100	25.510	10.857	-12.774	-1568.037
200	67.873	42.539	-7.954	-1571.507
298.15	91.881	74.559	0.	-1572.556
300	92.203	75.138	0.170	-1483.579
400	105.244	103.609	10.102	-1453.939
500	113.125	128.001	21.047	-1424.461
600	118.453	149.124	32.641	-1395.208
700	122.353	167.690	44.690	-1366.179
800	125.382	184.233	57.082	-1337.357
900	127.846	199.147	69.747	-1308.719
1000	129.938	212.728	82.639	-1279.523
1100	131.775	225.200	95.726	-1250.229
1200	133.432	236.738	108.987	-1220.909
1300	134.972	247.480	122.408	-1191.476
1400	136.423	257.536	135.979	-1159.002
1500	137.821	266.996	149.691	-1120.536
1600	139.185	275.934	163.542	-1082.079
1700	140.532	284.413	177.527	-1044.195
1800	141.879	292.483	191.748	-1006.291
1900	143.231	300.191	205.903	-968.533
1953.000	143.949	304.141	213.514	---
2000	144.595	307.572	220.294	-930.513
2100	145.980	314.660	234.873	-892.293
2200	147.194	321.484	249.491	-854.172
2300	148.333	328.067	264.307	-816.152
2400	150.310	334.433	279.259	-778.232
2500	151.825	340.599	294.366	-740.415
2600	153.381	346.584	309.626	-702.699
2700	154.975	352.402	325.033	-665.085
2800	156.615	358.068	340.622	-627.574
2900	158.302	363.593	356.368	-590.170
3000	160.038	368.989	372.284	-552.869

PREVIOUS: June 1961

CURRENT: June 1967

Magnesium Titanium Oxide (MgTiO₃)

Mg₁O₃Ti₁(cr)

Mg₃O₃Ti₄(l)Magnesium Titanium Oxide (MgTiO₃)M_r = 120.1832

LIQUID

Magnesium Titanium Oxide (MgTiO₃)

$S^{\circ}(298.15\text{ K}) = [111.082] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $T_{\text{fus}} = 1953 \pm 20 \text{ K}$

$$\Delta H_f^{\circ}(298.15\text{ K}) = [-1497.631 \pm 6.3] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_{\text{liq}}H_f^{\circ} = [90.374] \text{ kJ}\cdot\text{mol}^{-1}$$

Enthalpy of Formation
 $\Delta H_f^{\circ}(\text{MgTiO}_3, l, 298.15\text{ K})$ is calculated from $\Delta H_f^{\circ}(\text{MgTiO}_3, cr, 298.15\text{ K})$ by adding $\Delta_{\text{liq}}H_f^{\circ}$ and the difference in enthalpy, $H^{\circ}(1953\text{ K}) - H^{\circ}(298.15\text{ K})$, between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 1300 K. The heat capacity below 1300 K is obtained from the heat capacity of the crystal. Above 1300 K the heat capacity is assumed constant and estimated as $39 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ or $7.8 \text{ cal}\cdot\text{K}^{-1}\cdot\text{g}\cdot\text{atom}^{-1}$. $S^{\circ}(l, 298.15\text{ K})$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

The incongruent melting point is obtained from Massazza.¹ Previous work by Coughanour² indicates congruent melting point at 1903 K. The $\Delta_{\text{liq}}H_f^{\circ}$ is estimated from those of Na₂O 2TiO₂ and Na₂O TiO₂ observed by Naylor³ and CaO·TiO₂·SiO₂ observed by King.⁴

References

1. F. Massazza and E. Surchia, 16th Int Congress of Pure and Appl Chem., Inorg Sect., Paris (1957), pp 161-8, Butterworths Scientific Publications, London, (1958).
2. L. W. Coughanour and V. A. DeProse, J. Res. Nat. Bur. Stand. 51, 87 (1953).
3. B. F. Naylor, J. Amer. Chem. Soc. 67, 2120 (1945).
4. E. G. King, R. L. Orr and K. R. Bonnickson, J. Amer. Chem. Soc. 76, 4320 (1954).

T/K	C _p ^o	S ^o	-(G ^o -H ^o (T))/T	H ^o -H ^o (T)	Δ _{liq} H ^o	ΔG ^o	log K _r
0				0.			
100							
200							
298.15	91.881	111.082	111.082	111.082	-1497.631	-1420.091	248.794
300	92.203	111.651	111.083	111.083	-1497.635	-1419.610	247.176
400	105.244	140.132	114.878	10.102	-1497.329	-1393.623	181.988
500	113.123	164.524	122.479	12.047	-1496.378	-1367.797	142.893
600	118.453	185.647	131.245	32.641	-1495.117	-1342.196	116.849
700	122.353	204.213	140.370	44.690	-1493.710	-1316.819	88.262
800	125.382	220.756	149.403	57.082	-1492.236	-1291.649	64.336
900	127.846	235.670	158.173	69.747	-1490.789	-1266.664	43.515
1000	129.931	249.251	166.612	82.639	-1489.367	-1241.121	24.829
1100	131.775	261.723	174.699	95.726	-1488.990	-1215.479	5.718
1200	133.432	273.261	182.438	108.987	-1489.777	-1189.811	1.791
1300	134.972	284.003	189.842	122.409	-1496.342	-1164.030	46.771
1300.000	134.972	284.003	189.842	122.409	---	---	---
1300.000	163.176	284.003	189.842	122.409	---	---	---
1400	163.176	296.095	197.005	138.726	-1621.344	-1133.313	42.359
1500	163.176	307.353	203.991	155.044	-1615.717	-1100.794	38.333
1600	163.176	317.884	210.784	171.361	-1610.233	-1066.645	34.822
1700	163.176	327.771	217.378	187.679	-1604.905	-1032.535	31.735
1800	163.176	337.104	223.772	203.997	-1599.743	-999.334	29.000
1900	163.176	345.926	229.971	220.314	-1594.761	-966.115	26.560
1933.000	163.176	350.416	233.179	228.963	---	---	---
2000	163.176	354.296	235.980	236.632	-1604.658	-932.699	24.360
2100	163.176	362.258	241.805	252.949	-1600.872	-899.195	22.366
2200	163.176	369.848	247.454	269.267	-1597.010	-865.973	20.538
2300	163.176	377.102	252.953	285.585	-1593.251	-833.712	18.912
2400	163.176	384.047	258.254	301.902	-1589.518	-802.478	17.406
2500	163.176	390.708	263.420	318.220	-1585.818	-766.907	16.024
2600	163.176	397.108	268.439	334.537	-1582.152	-734.223	14.751
2700	163.176	403.266	273.320	350.855	-1578.520	-701.679	13.575
2800	163.176	409.200	278.067	367.173	-1574.922	-669.269	12.485
2900	163.176	414.926	282.688	383.490	-1571.357	-636.988	11.473
3000	163.176	420.458	287.189	399.808	-1567.828	-604.829	10.531
3100	163.176	425.809	291.575	416.125	-1564.332	-572.786	9.651
3200	163.176	430.989	295.851	432.443	-1560.871	-540.857	8.829
3300	163.176	436.011	300.023	448.761	-1557.446	-509.035	8.057
3400	163.176	440.882	304.094	465.078	-1554.057	-477.315	7.333
3500	163.176	445.612	308.070	481.396	-1550.706	-445.695	6.652
3600	163.176	450.209	311.955	497.713	-1547.392	-414.170	6.009
3700	163.176	454.680	315.752	514.031	-1544.117	-382.749	5.393
3800	163.176	459.031	319.466	530.349	-1540.887	-351.352	4.768
3900	163.176	463.270	323.099	546.666	-1537.700	-320.000	4.182
4000	163.176	467.401	326.655	562.984	-1534.557	-288.772	3.582
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PREVIOUS:

CURRENT: June 1967

Magnesium Titanium Oxide (MgTiO₃)Mg₃O₃Ti₄(l)

Mg₃Ti₂(cr,l) MgO₃Ti₂(cr,l)

Mg₂ = 120.1832 Magnesium Titanium Oxide (MgTiO₃)

0 to 1953 K crystal
above 1953 K liquid

Magnesium Titanium Oxide (MgTiO₃)

CRYSTAL-LIQUID

Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^o	S° - [G° - HF(T)]/T	H° - HF(T)	Δ _f H°	
0	0	INFINITE	-13.556	-1563.260	INFINITE
100	25.510	10.857	-12.774	-1541.350	805.119
200	67.873	42.539	-7.954	-1513.096	395.180
298.15	91.881	74.559	0	-1484.128	260.013
300	92.203	75.128	0.170	-1483.579	258.314
400	105.244	103.609	10.102	-1453.939	189.865
500	113.123	128.001	21.047	-1424.461	148.812
600	118.453	149.124	32.641	-1395.208	121.464
700	122.353	167.690	44.690	-1366.179	101.946
800	125.382	184.233	57.082	-1337.357	87.320
900	127.846	199.147	69.747	-1308.719	75.956
1000	129.938	212.728	82.639	-1279.523	66.835
1100	131.775	225.200	95.726	-1250.229	59.368
1200	133.432	236.738	108.987	-1220.909	53.145
1300	134.972	247.480	122.408	-1191.476	47.874
1400	136.423	257.536	135.979	-1161.902	43.243
1500	137.821	266.996	149.691	-1132.536	39.021
1600	139.185	275.934	163.542	-1102.979	35.333
1700	140.532	284.413	177.527	-1072.70	32.084
1800	141.879	292.483	191.648	-1041.193	29.202
1900	143.231	300.191	205.903	-1008.291	26.627
1953.000	143.949	304.141	213.514	-984.097	26.627
1953.000	163.176	350.416	303.888	CRYSTAL → LIQUID TRANSITION	
2000	163.176	354.296	311.557	-1604.658	24.360
2100	163.176	362.258	327.875	-1600.822	22.366
2200	163.176	369.848	344.193	-1597.019	20.558
2300	163.176	377.102	360.510	-1593.251	18.912
2400	163.176	384.047	376.828	-1589.518	17.406
2500	163.176	390.708	393.145	-1585.818	16.024
2600	163.176	397.108	409.463	-1582.152	14.751
2700	163.176	403.266	425.781	-1578.520	13.575
2800	163.176	409.100	441.998	-1574.922	12.485
2900	163.176	414.626	458.416	-1571.357	11.475
3000	163.176	420.458	474.733	-1567.828	10.551
3100	163.176	425.809	491.051	-1564.332	9.651
3200	163.176	430.989	507.369	-1560.871	8.829
3300	163.176	436.011	523.686	-1557.446	8.057
3400	163.176	440.882	540.004	-1554.057	7.333
3500	163.176	445.612	556.321	-1550.706	6.652
3600	163.176	450.209	572.639	-1547.392	6.009
3700	163.176	454.680	588.957	-1544.117	5.293
3800	163.176	459.031	605.274	-1540.879	4.568
3900	163.176	463.270	621.592	-1537.672	3.882
4000	163.176	467.401	637.909	-1534.504	3.232

PREVIOUS:

CURRENT: June 1967

Magnesium Titanium Oxide (MgTiO₃)

Mg₃O₃Ti₂(cr,l)

Mg₁O₄S₁(cr)Magnesium Sulfate (MgSO₄)M_r = 120.3626

CRYSTAL

Magnesium Sulfate (MgSO₄)

S^o(298.15 K) = 91.40 ± 0.8 J·K⁻¹·mol⁻¹
 T_{fus} = 1400 K

ΔH^of(0 K) = -1250.40 ± 20.9 kJ·mol⁻¹
 ΔH^of(298.15 K) = -1261.79 ± 20.9 kJ·mol⁻¹
 Δ_{ion}H^o = 14 644 kJ·mol⁻¹

Enthalpy of Formation

The adopted Δ_fH^o(298.15 K) = -301.6 ± 5 kcal·mol⁻¹ was calculated from the Δ_fH^o(298.15 K) = 63.3 ± 5 kcal·mol⁻¹ for the reaction MgO(cr) + SO₃(g) = MgSO₄(cr). The value of Δ_fH^o(298.15 K) was calculated by the 3rd law method using the equilibrium data obtained from a transpiration study by Knopf and Staudt.¹ In addition Marchal² measured the total pressure of SO₃(g), SO₂(g) and O₂(g) above MgSO₄(cr) and partial pressures were obtained by application of the SO₂-SO₃ equilibrium data. Another value of Δ_fH^o(MgSO₄, cr, 298.15 K) may be derived from the measured enthalpy of solution of MgSO₄(cr) by Thomsen³ and the measured enthalpies of mixing of MgCl₂(aq, 200 H₂O) with H₂SO₄(aq, 200 H₂O) and MgSO₄(aq, 200 H₂O) with 2HCl(100 H₂O) by Thomsen.⁴

Source	Reaction	T/K	Drift cal·K ⁻¹ ·mol ⁻¹	Δ _f H ^o (298.15 K) kcal·mol ⁻¹	Δ _f H ^o (298.15 K) kcal·mol ⁻¹
1	MgO(cr) + SO ₃ (g) = MgSO ₄ (cr)	1144-1313	0.514	63.284	-301.574
2	MgO(cr) + SO ₃ (g) = MgSO ₄ (cr)	1223-1428	0.525	72.394	-310.867
3	MgSO ₄ (cr) = MgSO ₄ (aq, 200 H ₂ O)	298.15	-20.84		
4	MgCl ₂ (aq, 200 H ₂ O) + H ₂ SO ₄ (aq, 200 H ₂ O) = MgSO ₄ (aq, 200 H ₂ O) + 2HCl(aq, 100H ₂ O)	298.15		-3.52	-305.1*

*Combination of the reactions 3 and 4 with the following Δ_fH^o(298.15 K):

H₂SO₄(aq, 200 H₂O) = -212.387, HCl(aq, 100 H₂O) = -39.74 and MgCl₂(aq, 200 H₂O) = -189.5 kcal·mol⁻¹.

Heat Capacity and Entropy

The low temperature heat capacities 53.3-295.4 K were measured by Moore and Kelley.⁴ The heat capacities in the temperature range 298-1400 K were estimated from the equation MgSO₄(cr) = CaSO₄(cr) + MgO(cr) - CaO(cr) CaSO₄(cr) and CaO(cr) C_p^o were calculated using the equation C_p^o = 16.78 + 23.60 × 10⁻³T and C_p^o = 11.67 + 1.08 × 10⁻³T - 1.56 × 10⁻⁷T² respectively, Kelley.⁵ The heat capacity of MgO(cr) was calculated from the correlation of the low temperature heat capacities. The values from the two sources join smoothly at 298.15 K. Above the melting point (1400 K) the heat capacity was graphically extrapolated. The entropy was calculated at 50.12 K using the Debye and Einstein function D(242/T) + 2E(378/T) + 2E(866/T) + E(1683/T) given by Moore and Kelley.⁴ The value of S^o(50.12 K) = 1.08 cal·K⁻¹·mol⁻¹.

Fusion Data

T_{fus} and Δ_{ion}H^o from Kelley.⁶

References

- H. J. Knopf and H. Staudt, Z. Physik. Chem. (Leipzig) 204, 265 275 (1955).
- G. Marchal, J. Chim. Phys. 22, 493 (1925).
- J. Thomsen, "Thermochemische Untersuchungen," Vols. I IV, Barth, Leipzig (1882-1886).
- G. E. Moore and K. K. Kelley, J. Amer. Chem. Soc. 64, 2949 (1942).
- K. K. Kelley, U. S. Bur. Mines Bull. 584, (1960).
- K. K. Kelley, U. S. Bur. Mines Bull. 393, (1936).

Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p ^o = 0.1 MPa				
T/K	C _p ^o J·K ⁻¹ ·mol ⁻¹	S ^o - (C _p ^o - H ^o (T _r))/T _r	H ^o - H ^o (T _r) kJ·mol ⁻¹	Δ _f H ^o kJ·mol ⁻¹	ΔG ^o	log K _f
0	0	INFINITE	-15.390	-1250.399	-1250.399	INFINITE
100	36.313	19.979	-14.032	-1256.182	-1221.316	637.950
200	73.309	51.532	-8.400	-1260.022	-1184.778	309.432
298.15	96.232	91.396	0	-1261.786	-1147.408	201.021
300	96.441	91.398	0.178	-1261.804	-1146.698	199.658
400	109.997	121.692	10.535	-1264.542	-1108.138	144.708
500	119.411	147.271	22.015	-1265.774	-1068.894	111.667
600	127.612	169.790	34.379	-1266.082	-1029.474	89.624
700	134.306	189.970	47.479	-1265.710	-990.061	71.879
800	140.499	208.314	61.223	-1264.839	-950.737	62.077
900	146.231	225.196	75.562	-1316.686	-910.467	52.842
1000	151.670	240.888	90.461	-1322.424	-864.769	45.171
1100	156.691	255.582	105.881	-1319.324	-819.150	38.898
1200	161.419	269.424	121.793	-1315.827	-773.831	33.684
1300	165.352	282.504	138.137	-1311.983	-728.819	29.284
1400	168.619	294.881	154.840	-1435.265	-680.946	25.406
1400.000	168.619	294.882	154.841	---	CRYSTAL < -> LIQUID	---
1500	171.389	306.611	171.843	-1429.556	-627.265	21.843
1600	173.787	317.750	189.105	-1423.656	-573.970	18.738
1700	175.895	328.350	206.591	-1417.595	-521.049	16.010
1800	177.778	338.458	224.276	-1411.397	-468.490	13.595
1900	179.477	348.117	242.140	-1405.080	-416.278	11.444
2000	181.033	357.363	260.166	-1398.658	-364.401	9.517
2100	182.468	366.230	278.342	-1392.145	-312.848	7.782
2200	183.807	374.750	296.657	-1385.549	-261.606	6.211
2300	185.067	382.949	315.101	-1378.878	-210.606	4.784
2400	186.259	390.850	333.668	-1372.138	-160.021	3.483
2500	187.393	398.477	352.351	-1365.335	-109.656	2.291

PREVIOUS: December 1960

CURRENT: March 1966

Magnesium Sulfate (MgSO₄)Mg₁O₄S₁(cr)

Magnesium Sulfate (MgSO₄)

Magnesium Sulfate (MgSO₄)

LIQUID

Magnesium Sulfate (MgSO₄)

Mg₃O₄S₃(l)

$S^\circ(298.15\text{ K}) = [102.125] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $T_{\text{fus}} = 1400\text{ K}$
 $\Delta_f H^\circ(298.15\text{ K}) = [-1246.587] \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{liq}} H^\circ = 14.644 \text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation
 $\Delta_f H^\circ(\text{MgSO}_4, l, 298.15\text{ K})$ is calculated from $\Delta_f H^\circ(\text{MgSO}_4, \text{cr}, 298.15\text{ K})$ by adding $\Delta_{\text{liq}} H^\circ$ and the difference in enthalpy, $H^\circ(1400\text{ K}) - H^\circ(298.15\text{ K})$, between the crystal and liquid.

Heat Capacity and Entropy
 A glass transition was assumed at 1000 K. The heat capacity below 1000 K was obtained from the heat capacity of the crystal. Above 1000 K the heat capacity was assumed constant and estimated as $38.0 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ by comparison with those for $\text{MgCl}_2(l)$, $\text{KCl}(l)$ and $\text{K}_2\text{SO}_4(l)$. $S^\circ(l, 298.15\text{ K})$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data
 Refer to the crystal table for details.

T/K	C _p ^o	Enthalpy Reference Temperature = T, = 298.15 K		H ^o - H ^o (T ₁)	Δ _f H ^o	Δ _g G ^o	log K _f
		S ^o - [S ^o - H ^o (T ₁)]/T	kJ·mol ⁻¹				
0							
100							
200							
298.15	96.232	102.125	102.125	0.	-1246.587	-1135.408	198.919
300	96.441	102.721	102.127	0.178	-1246.605	-1134.718	197.572
400	109.997	132.421	106.084	10.535	-1249.343	-1097.231	143.284
500	119.411	158.000	113.970	22.015	-1250.575	-1059.059	110.639
600	127.612	180.519	123.221	34.379	-1250.883	-1020.713	88.861
700	134.306	200.700	132.873	47.479	-1250.511	-982.373	73.306
800	140.499	219.043	142.514	61.223	-1249.640	-944.122	61.645
900	146.231	235.858	151.964	75.505	-1301.545	-904.921	52.520
1000	158.574	251.845	161.156	90.690	-1306.996	-860.299	44.937
1000.000	158.574	251.845	161.156	90.690	GLASS <- -> LIQUID		
1000.000	158.992	251.845	161.156	90.690	TRANSITION		
1100	158.992	266.999	170.100	106.589	-1303.417	-815.802	38.739
1200	158.992	280.833	178.760	122.488	-1299.933	-771.628	33.588
1300	158.992	293.559	187.108	138.387	-1296.534	-727.741	29.241
1400	158.992	305.342	195.137	154.286	-1420.620	-680.946	25.406
1400.000	158.992	305.342	195.137	154.286	CRYSTAL <- -> LIQUID		
1500	158.992	316.311	202.854	170.186	-1416.015	-628.274	21.878
1600	158.992	326.572	210.269	186.085	-1411.477	-575.906	18.801
1700	158.992	336.211	217.397	201.984	-1407.003	-523.820	16.095
1800	158.992	345.299	224.253	217.883	-1402.590	-471.996	13.697
1900	158.992	353.895	230.852	233.782	-1398.238	-420.415	11.558
2000	158.992	362.050	237.209	249.682	-1393.944	-369.062	9.639
2100	158.992	369.808	243.340	265.581	-1389.707	-317.923	7.908
2200	158.992	377.204	249.258	281.480	-1385.526	-266.982	6.339
2300	158.992	384.271	254.976	297.379	-1381.400	-216.233	4.911
2400	158.992	391.038	260.505	313.278	-1377.328	-165.662	3.606
2500	158.992	397.528	265.857	329.178	-1373.310	-115.258	2.408

PREVIOUS: December 1960

CURRENT: March 1965

Magnesium Sulfate (MgSO₄)

Mg₃O₄S₃(l)

Magnesium Sulfate (MgSO₄)

CRYSTAL-LIQUID

M_r = 120.3626 Magnesium Sulfate (MgSO₄)Mg₁₀O₄S₁(cr,l)

0 to 1400 K crystal
above 1400 K liquid

Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^a	S° - [G° - H°(T _r)]/T	H° - H°(T _r)	ΔH°	
	J·K ⁻¹ ·mol ⁻¹	J·K ⁻¹ ·mol ⁻¹	J·mol ⁻¹	kJ·mol ⁻¹	
0	0	0	INFINITE	-1250.399	INFINITE
100	36.313	19.979	160.297	-1251.316	637.950
200	73.369	57.552	99.534	-1184.778	309.432
298.15	96.232	91.396	91.396	-1147.408	201.021
300	96.441	91.992	91.398	-1146.698	199.658
400	109.997	121.692	95.355	-1108.138	144.708
500	119.411	147.271	103.240	-1068.894	111.667
600	127.612	169.790	112.492	-1029.474	89.624
700	134.368	189.970	122.143	-990.061	73.879
800	140.499	208.314	131.785	-950.737	62.077
900	146.231	225.196	141.238	-910.467	52.842
1000	151.670	240.868	150.428	-864.769	43.171
1100	156.691	255.582	159.376	-819.150	38.898
1200	161.419	269.424	167.930	-773.831	33.684
1300	165.352	282.504	176.245	-728.819	29.284
1400	168.619	294.882	184.281	-680.946	25.406
1400.000	168.619	294.882	184.281	-680.946	25.406
1400.000	158.992	305.342	184.281	CRYSTAL ← → LIQUID TRANSITION	
1500	158.992	316.311	192.721	-1416.015	21.878
1600	158.992	326.572	200.770	-1411.477	18.801
1700	158.992	336.211	208.456	-1407.003	16.095
1800	158.992	345.299	215.809	-1402.590	13.697
1900	158.992	353.895	222.852	-1398.238	11.558
2000	158.992	362.050	229.610	-1393.944	9.639
2100	158.992	369.898	236.103	-1389.707	7.908
2200	158.992	377.204	242.350	-1385.576	6.339
2300	158.992	384.271	248.368	-1381.400	4.911
2400	158.992	391.038	254.172	-1377.328	3.606
2500	158.992	397.528	259.778	-1373.310	2.408

PREVIOUS:

CURRENT: March 1966

Magnesium Sulfate (MgSO₄)Mg₁₀O₄S₁(cr,l)

Mg₃O₄W₄(cr)

Magnesium Tungsten Oxide (MgWO₄)

CRYSTAL

Magnesium Tungsten Oxide (MgWO₄)

M_r = 272.1526

$\Delta_f H^\circ(0 \text{ K}) = -1505.74 \pm 33.5 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_f H^\circ(298.15 \text{ K}) = -1515.86 \pm 33.5 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{ref}} H^\circ = \text{Unknown}$

Enthalpy of Formation

Rezukhina and Levitskii¹ measured the emf, $E = 0.2433 - 0.00012647T$, for the cell reaction $\text{MgO}(\text{cr}) + \text{W}(\text{cr}) + 3\text{Fe}_{0.95}\text{O}(\text{cr}) = \text{MgWO}_4(\text{cr}) + 2.85 \text{ Fe}(\text{cr})$ in the temperature range 1220–1370 K. Incorporating the results with auxiliary thermal data, the authors obtained $\Delta_f G^\circ = -224.370 + 65.677T$ (cal·K⁻¹·mol⁻¹) for $\text{MgO}(\text{cr}) + \text{W}(\text{cr}) + 3/20(\text{g}) \rightarrow \text{MgWO}_4(\text{cr})$. 3rd law analysis of the $\Delta_f G^\circ$ equation gives $\Delta_f H^\circ(298.15 \text{ K}) = -218.6 \text{ kcal}\cdot\text{mol}^{-1}$, from which the adopted $\Delta_f H^\circ(\text{MgWO}_4, \text{cr}, 298.15 \text{ K}) = -362.3 \text{ kcal}\cdot\text{mol}^{-1}$, is calculated. The 2nd law analysis gives $\Delta_f H^\circ(\text{MgWO}_4, \text{cr}, 298.15 \text{ K}) = -372.7 \text{ kcal}\cdot\text{mol}^{-1}$. The drift is 8.0 cal·K⁻¹·mol⁻¹.
 Rezukhina, *et. al.*² determined the Gibbs energy changes $\Delta_f G^\circ = 51,300 - 27.677T$ (cal·K⁻¹·mol⁻¹) for the reaction $\text{MgWO}_4(\text{cr}) + 3\text{H}_2(\text{g}) \rightarrow \text{MgO}(\text{cr}) + \text{W}(\text{cr}) + 3\text{H}_2\text{O}(\text{g})$ in the temperature range 1073 K–1273 K by a circulation method. This leads to heats of formation of 366.1 kcal·mol⁻¹ by the 3rd law method and 377.2 kcal·mol⁻¹ by the 2nd law method. Both determinations were performed by Rezukhina and his co workers, but they considered the data obtained by the emf method to be more reliable than that derived from heterogeneous equilibria.

Heat Capacity and Entropy

Low temperature heat capacities, 52.92–296.09 K, were measured calorimetrically by King and Weller.³ The heat capacities above 300 K are estimated by comparison with those of CaWO₄(cr),⁴ CaO(cr),⁵ and MgO(cr).⁶ These two sets of data are joined smoothly at 298.15 K by a graphical method.

The entropy, $S^\circ(298.15 \text{ K}) = 21.184 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$, is taken from King and Weller,³ based on an extrapolation of $S^\circ(51 \text{ K}) = 1.27 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$. No spin magnetic entropy is predicted below 51 K based on the diamagnetism observed by Gerasimov.⁷

References

- ¹T. N. Rezukhina and V. A. Levitskii, Russ. J. Phys. Chem. **37**, 1277 (1963).
- ²T. N. Rezukhina, Ya. I. Gerasimov and Yu. P. Simanov, Vesnik Moskov Univ. **4**, No 6, 103 (1949).
- ³E. G. King and W. W. Weller, U. S. Bur. Mines RI 5791, (1961).
- ⁴R. A. Yakovleva and T. N. Rezukhina, Russ. J. Phys. Chem. **34**, 390 (1960).
- ⁵K. K. Kelley, U.S. Bur. Mines Bull. **584**, (1960).
- ⁶JANAF Thermochemical Tables: MgO, 12–31–65.
- ⁷Ya. I. Gerasimov, Papers Presented to Section on Inorganic Chemistry, 16th Intern. Congress Pure and Applied Chem. Paris (1957), pp. 227–35, Butterworths Scientific Publications, London, (1958).

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^o	S° - (G° - H°(T _r))/T	H° - H°(T _r)/T	Δ _r H°	
0	0	0	INFINITE	-1505.744	INFINITE
100	38.221	21.150	179.146	-1511.429	771.490
200	83.220	62.706	110.418	-1515.008	376.317
298.15	109.077	101.186	0	-1515.863	246.014
300	109.621	101.862	0.202	-1404.224	244.377
400	123.428	133.424	105.670	-1515.122	178.464
500	131.587	163.893	114.543	-1515.648	138.849
600	137.026	188.377	124.856	-1511.854	112.509
700	141.670	209.851	135.496	-1509.900	93.718
800	146.147	229.063	146.011	-1507.815	79.643
900	150.415	246.522	156.223	-1505.606	68.712
1000	154.808	262.595	166.067	-1511.860	59.943
1100	159.410	277.566	175.530	-1509.378	52.769
1200	164.013	291.633	184.625	-1506.559	46.801
1300	168.615	304.945	193.373	-1503.393	41.762
1400	173.008	317.600	201.798	-1500.027	37.334
1500	177.611	329.694	209.924	-1496.488	33.292
1600	182.004	341.296	217.775	-1492.823	29.768
1700	186.606	352.469	225.371	-1489.066	26.669
1800	191.000	363.259	232.734	-1485.255	23.925
1900	195.602	373.710	239.880	-1481.302	21.479
2000	199.595	383.835	246.826	-1477.254	19.288

PREVIOUS: June 1963

CURRENT: March 1967

Magnesium Tungsten Oxide (MgWO₄)

Mg₃O₄W₄(cr)

Magnesium Titanium Oxide (MgTi₂O₃)

Mg₂O₃Ti₂(cr)

Mg₂O₃Ti₂(cr)

T/K	C _p ^o	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p ^o = 0.1 MPa		log K _f
		S ^o - (G ^o - H ^o (T _r))/T _r	H ^o - H ^o (T _r)	ΔH ^o	ΔG ^o	
0	0	INFINITE	-22.439	-2495.427	INFINITE	
100	46.129	22.217	-20.891	-2459.195	1284.552	
200	110.533	75.538	-12.811	-2413.208	630.265	
298.15	146.858	135.603	0	-2368.790	415.002	
300	147.335	135.606	0.272	-2367.918	412.291	
400	165.753	181.688	16.019	-2320.819	303.068	
500	176.665	219.925	33.175	-2273.965	237.559	
600	184.498	252.858	51.250	-2227.426	193.915	
700	190.807	281.785	70.074	-2181.202	162.763	
800	196.276	307.628	89.383	-2135.276	139.419	
900	201.238	331.036	109.262	-2089.630	121.279	
1000	205.870	352.481	129.620	-2043.521	106.743	
1100	210.284	372.311	150.479	-2003.688	94.849	
1200	214.539	390.791	171.671	-1971.403	84.934	
1300	218.681	408.127	193.332	-1946.427	76.536	
1400	222.739	424.482	215.404	-1926.346	69.229	
1500	226.731	439.986	237.878	-1910.324	62.693	
1600	230.672	454.747	260.748	-1897.488	56.984	
1700	234.572	468.847	284.011	-1886.831	51.959	
1800	238.438	482.364	307.662	-1877.711	47.498	
1900	242.279	495.359	331.698	-1869.861	43.516	
1963.000	244.685	503.301	347.037	-1863.324	39.916	
2000	246.099	507.883	329.825	-1858.493	36.649	
2100	249.902	519.982	338.593	-1854.683	33.684	
2200	253.698	531.695	347.106	-1851.979	30.981	
2300	257.458	543.095	355.380	-1850.348	28.507	
2400	261.270	554.092	363.511	-1849.771	26.236	
2500	264.973	564.832	371.273	-1850.251	24.144	
2600	268.713	575.237	378.919	-1851.818	22.211	
2700	272.450	585.508	386.383	-1854.473	20.470	
2800	276.177	595.484	393.673	-1858.221	18.756	
2900	279.901	605.241	400.801	-1863.067	17.208	
3000	283.621	614.792	407.775	-1868.992		

PREVIOUS: June 1961

CURRENT: June 1967

Magnesium Titanium Oxide (MgTi₂O₃)

Mg₂O₃Ti₂(cr)

Mg₂O₃Ti₂(cr)

$S^{\circ}(298.15\text{ K}) = 135.60 \pm 6.3\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $T_{\text{fus}} = 1963 \pm 20$

Enthalpy of Formation
 $\Delta H_f^{\circ}(298.15\text{ K})$ is calculated from $\Delta H_f^{\circ}(298.15\text{ K}) = -4.45 \pm 0.45\text{ kcal}\cdot\text{mol}^{-1}$ for the reaction $\text{MgO}(\text{cr}) + 2\text{TiO}_2(\text{rutile}) = \text{MgTi}_2\text{O}_3(\text{cr})$ measured by Kelley *et al.*,¹ using a solution calorimetric method. The uncertainty of $\pm 2.5\text{ kcal}\cdot\text{mol}^{-1}$ assigned to the enthalpy of formation is due primarily to $\text{TiO}_2(\text{rutile})$.

Heat Capacity and Entropy
 Low temperature heat capacities are from the data (52–296 K) of Todd.² High temperature enthalpies have been measured (397–1812 K) by Orr and Coughlin.³ High temperature heat capacities are derived from the enthalpies by a fitting technique which constrains the curve to join smoothly with the low temperature values. The entropy is based on $S^{\circ}(51\text{ K}) = 1.11\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$.

Kelley *et al.*,¹ suggested that there may be a zero-point entropy due to randomness of the cations. The authors estimated $S^{\circ}(0\text{ K})$ from the following alternative assumptions (a) all the Mg and Ti ions are randomly distributed among the lattice sites giving $3.79\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ and (b) all the Mg and one-half of the Ti ions are randomly distributed giving $2.75\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$. These assumptions were proposed in order to make MgTi_2O_3 stable relative to MgTiO_3 at high temperatures. Phase data of Massazza and Sirchia,⁴ indicate that MgTi_2O_3 melts congruently at $1963 \pm 20\text{ K}$ and that there is a temperature range. To make $\Delta_f G^{\circ}(1800\text{ K}) < 0$ would require that $S^{\circ}(0\text{ K}) \geq 0.35\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$. We adopt a compromise zero-point entropy of $2\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ between the upper ($3.79\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) and the lower ($0.35\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$) limits.

Fusion Data

Refer to the liquid table for details.

References

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Mg₁O₂Ti₂(l) Mg₁O₂Ti₂(l)

T/K	C _p ^o	S ^o - [G ^o - H ^o (T)]/T	H ^o - H ^o (T)	Δ _f H ^o	log K _r
0			0		
100					
200					
298.15	146.858	197.783	197.783	-2382.307	395.992
300	147.335	198.692	197.785	-2382.310	399.418
400	165.733	243.867	203.819	-2381.773	289.725
500	176.665	282.105	215.754	-2380.411	227.535
600	184.498	315.037	229.620	-2378.654	186.102
700	190.807	343.964	243.931	-2376.665	156.531
800	196.276	369.807	258.078	-2374.486	134.372
900	201.238	393.215	271.813	-2372.221	117.153
1000	205.870	414.660	285.040	-2370.616	103.354
1100	210.284	434.690	297.736	-2376.641	92.064
1200	214.539	452.970	309.911	-2382.691	82.652
1300	218.681	470.307	321.589	-2379.379	74.679
1300.000	218.681	470.307	321.589	193.333	
1300.000	261.082	470.307	321.589	193.333	
1400	261.082	489.655	332.911	219.441	67.743
1500	261.082	507.668	343.968	245.549	61.537
1600	261.082	524.518	354.732	271.657	56.125
1700	261.082	540.345	365.189	297.765	51.166
1800	261.082	555.268	375.339	323.873	47.149
1900	261.082	569.384	385.184	349.982	43.387
1963.000	261.082	577.901	391.233	366.490	40.000
2000	261.082	582.776	394.731	376.090	39.988
2100	261.082	595.514	403.992	402.198	36.905
2200	261.082	607.660	412.975	428.306	34.108
2300	261.082	619.265	421.699	454.414	31.159
2400	261.082	630.377	430.159	480.522	29.228
2500	261.082	641.035	438.383	506.631	27.087
2600	261.082	651.275	446.375	532.739	25.115
2700	261.082	661.128	454.148	558.847	23.293
2800	261.082	670.623	461.710	584.955	21.604
2900	261.082	679.783	469.073	611.063	20.034
3000	261.082	688.636	476.245	637.171	18.572
3100	261.082	697.196	483.235	663.280	17.207
3200	261.082	705.485	490.052	689.388	15.930
3300	261.082	713.519	496.702	715.496	14.732
3400	261.082	721.313	503.195	741.604	13.605
3500	261.082	728.882	509.535	767.712	12.547
3600	261.082	736.236	515.731	793.820	11.549
3700	261.082	743.390	521.788	820.928	10.586
3800	261.082	750.352	527.711	848.037	9.691
3900	261.082	757.134	533.507	875.145	8.860
4000	261.082	763.744	539.181	902.253	8.067

PREVIOUS: June 1961 CURRENT: June 1967

Magnesium Titanium Oxide (MgTi₂O₅) Mg₁O₂Ti₂(l)

$S^{\circ}(298.15\text{ K}) = [197.783] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $T_{\text{fus}} = 1963 \pm 20 \text{ K}$
 $\Delta_f H^{\circ}(298.15\text{ K}) = [-2382.31 \pm 8.4] \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{fus}} H^{\circ} = [146.440] \text{ kJ}\cdot\text{mol}^{-1}$

LIQUID
M_f = 200.0620
Magnesium Titanium Oxide (MgTi₂O₅)
 Enthalpy of Formation
 $\Delta_f H^{\circ}(\text{MgTi}_2\text{O}_5, l, 298.15\text{ K})$ is calculated from $\Delta_f H^{\circ}(\text{MgTi}_2\text{O}_5, \text{cr}, 298.15\text{ K})$ by adding $\Delta_{\text{fus}} H^{\circ}$ and the difference in enthalpy, $H^{\circ}(1963\text{ K}) - H^{\circ}(298.15\text{ K})$, between the crystal and liquid.

Heat Capacity and Entropy
 A glass transition is assumed at 1300 K. Below 1300 K the heat capacity is obtained from the heat capacity of the crystal. Above 1300 K the heat capacity is assumed constant and estimated as $62.4 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ or $7.8 \text{ cal}\cdot\text{K}^{-1}\cdot\text{g}\cdot\text{atom}^{-1}$. $S^{\circ}(l, 298.15\text{ K})$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data
 The congruent melting point is obtained from Massazza.¹ Previous work by Coughanour² indicates congruent melting at 1925 K. The $\Delta_{\text{fus}} H^{\circ}$ is estimated from those of Na₂O 2TiO₂ and Na₂O·TiO₂ observed by Naylor³ and CaO·TiO₂·SiO₂ observed by King.⁴

References
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²L. W. Coughanour and V. A. DeProse, J. Res. Nat. Bur. Stand. 51, 87 (1953).
³B. V. Naylor, J. Amer. Chem. Soc. 67, 2120 (1945).
⁴E. G. King, R. L. Orr and K. R. Bonnickson, J. Amer. Chem. Soc. 76, 4320 (1954).

Magnesium Titanium Oxide (MgTi₂O₃) CRYSTAL-LIQUID

M_r = 200.0620 Magnesium Titanium Oxide (MgTi₂O₃)

Mg₃O₅Ti₂(cr,l)

0 to 1963 K crystal
above 1963 K liquid

Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^o	S° - [C _p ^o - H ^o (T _r)]/T	H° - H ^o (T _r)	Δ _r G°	
		J·K ⁻¹ ·mol ⁻¹	J·mol ⁻¹	KJ·mol ⁻¹	
0	0	INFINITE	-22.439	-2495.427	INFINITE
100	46.129	22.217	-20.891	-2459.195	1284.552
200	110.533	75.638	-12.811	-2413.208	630.265
298.15	146.858	135.603	0	-2368.790	415.002
300	147.335	136.513	0.272	-2367.918	412.291
400	165.753	181.688	16.019	-2320.819	303.068
500	176.665	219.925	33.175	-2273.965	237.559
600	184.498	252.858	51.250	-2205.701	193.915
700	190.807	281.785	70.024	-2118.202	162.763
800	196.276	307.628	89.383	-2015.276	139.419
900	201.238	331.036	109.262	-2089.630	121.279
1000	205.870	352.481	129.670	-2043.521	106.743
1100	210.284	372.311	150.429	-1997.403	94.849
1200	214.539	390.791	171.671	-1951.222	84.934
1300	218.681	408.127	193.332	-1904.812	76.536
1400	222.739	424.482	215.404	-1855.496	69.229
1500	226.751	439.986	237.878	-1803.324	62.693
1600	230.672	454.745	260.748	-1745.488	56.984
1700	234.572	468.847	284.011	-1690.975	51.957
1800	238.438	482.364	307.562	-1636.771	47.498
1900	242.279	495.359	331.698	-1582.861	43.516
1963.000	244.685	503.301	347.037	-1531.089	39.988
1963.000	261.082	577.901	493.477	-1483.696	36.905
2000	261.082	582.776	503.137	-1483.696	36.905
2100	261.082	595.514	529.245	-1436.544	34.108
2200	261.082	607.660	555.353	-1389.624	31.559
2300	261.082	619.265	581.462	-1342.919	29.228
2400	261.082	630.377	607.570	-1296.419	27.087
2500	261.082	641.035	633.678	-1250.113	25.115
2600	261.082	651.275	659.786	-1203.892	23.293
2700	261.082	661.128	685.894	-1158.047	21.604
2800	261.082	670.623	712.002	-1112.272	20.034
2900	261.082	679.785	738.110	-1066.655	18.572
3000	261.082	688.656	764.219	-1021.190	17.207
3100	261.082	697.196	790.327	-975.875	15.930
3200	261.082	705.485	816.435	-930.700	14.732
3300	261.082	713.519	842.543	-885.656	13.606
3400	261.082	721.313	868.651	-840.744	12.547
3500	261.082	728.882	894.759	-795.954	11.549
3600	261.082	736.236	920.868	-753.708	10.586
3700	261.082	743.390	946.976	-713.497	9.191
3800	261.082	750.352	973.084	-668.648	8.060
3900	261.082	757.134	999.192	-601.763	6.987
4000	261.082	763.744	1025.300	-535.044	

PREVIOUS

CURRENT, June 1967

Magnesium Titanium Oxide (MgTi₂O₃)

Mg₃O₅Ti₂(cr,l)

Magnesium Sulfide (MgS)

M_f = 56.365 Magnesium Sulfide (MgS)

Mg₃S₄(cr)

S°(298.15 K) = 50.33 ± 0.4 J·K⁻¹·mol⁻¹ ΔH_f°(0 K) = -344.65 ± 4.2 kJ·mol⁻¹ ΔH_f°(298.15 K) = -345.72 ± 4.2 kJ·mol⁻¹

Enthalpy of Formation

Sabatier¹ determined ΔH_f°(286 K) = -37.8 ± 1.0 kcal·mol⁻¹ while Moutlot² determined ΔH_f°(291 K) = -38.0 ± 1.0 kcal·mol⁻¹ for MgS(cr) + 2 HCl(aq, 100 H₂O) → MgCl₂(aq, 100 H₂O) + H₂S(aq). We derive ΔH_f°(MgS, cr, 298.15 K) = -83.0 ± 2.0 kcal·mol⁻¹ and ΔH_f°(MgS, cr, 298.15 K) = 82.8 ± 2.0 kcal·mol⁻¹, respectively based on the following auxiliary data: ΔH_f°(HCl, 100 H₂O, aq, 298.15 K) = -39.657 kcal·mol⁻¹, ΔH_f°(H₂S, aq, 298.15 K) = -9.5 kcal·mol⁻¹, and ΔH_f°(MgCl₂, 100 H₂O, aq, 298.15 K) = -190.59 kcal·mol⁻¹. The uncertainty reflects the correction to 298.15 K and the ambiguity of the exact solution composition. Von Wartenberg³ measured ΔH_f°(293 K) = -33.95 ± 0.79 kcal·mol⁻¹ for MgS(cr) + 2 HCl(30 H₂O, aq) → MgCl₂(30 H₂O, aq) + H₂S(g). We derive ΔH_f°(MgS, cr, 298.15 K) = -82.0 ± 1.0 kcal·mol⁻¹ based on the following auxiliary data: ΔH_f°(HCl, 30 H₂O, aq, 298.15 K) = 39.357 kcal·mol⁻¹, ΔH_f°(H₂S, g, 298.15 K) = -4.90 kcal·mol⁻¹, and ΔH_f°(MgCl₂, 30 H₂O, aq, 298.15 K) = 189.78 kcal·mol⁻¹. Kapustinskii and Korshunov⁴ performed calorimetric measurements of the enthalpy of formation of MgS(cr) from the pure elements. They determined ΔH_f°(298.15 K) = -84.33 ± 0.27 kcal·mol⁻¹ for Mg(cr) + S(cr, rhombic) = MgS(cr).

Our analyses of equilibrium studies of Curlock and Pidgeon⁵ and of Dewing and Richardson⁶ are given below. The two studies are in reasonable agreement. The 3rd law ΔH_f°(298.15 K) may be in error by as much as 0.5 kcal·mol⁻¹ since the Gibbs energy functions employed in the calculations are partially based on estimated high temperature C_p° values.

Source	Method	Data Points	Reaction ^a	T/K	ΔS cal·K ⁻¹ ·mol ⁻¹	ΔH _f °(298.15 K), kcal·mol ⁻¹	ΔH _f °(298.15 K), kcal·mol ⁻¹
Curlock ⁵	Equilibrium	6	A	1180-1483	-0.60 ± 0.45	-8.49 ± 0.59	-9.19 ± 0.24
Dewing ⁶	Equilibrium	6	A	1267-1768	-2.23 ± 0.22	-5.53 ± 0.38	-8.73 ± 1.01

^aReaction: A) MgS(cr) + H₂O(g) = MgO(cr) + H₂S(g)

Our adopted value is based on a weighted average of all the data.

Heat Capacity and Entropy

Stull *et al.*⁷ measured the low temperature heat capacities in an adiabatic calorimeter from 15-320 K. Their smooth values are adopted in the tabulation. The entropy S°(298.15 K) = 12.03 ± 0.1 cal·K⁻¹·mol⁻¹ is based on S° = 0.010 cal·K⁻¹·mol⁻¹ at 15 K.⁸ The C_p° values above 320 K are estimated by graphical extrapolation combined with method B of Kubaschewski *et al.*¹⁰

Fusion Data

MgS melts above 2300 K¹¹ and no other literature melting data are available.

References

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T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K _r
	C _p ^o	S° - (G° - (T _r T))/T	H° - H°(T _r)	ΔH _f °	
0	0	0	INFINITE	-344.647	INFINITE
100	22.677	10.920	86.467	-344.200	179.734
200	40.125	33.095	54.342	-345.544	89.532
298.15	45.564	50.334	0	-345.724	59.818
300	45.647	50.334	0.084	-341.433	59.444
400	47.614	64.037	57.150	-348.212	44.379
500	48.955	74.807	55.639	-349.975	35.264
600	49.915	83.823	59.606	-351.381	29.159
700	50.543	91.566	63.631	-352.575	24.781
800	51.003	98.346	67.556	-353.697	21.488
900	51.463	104.380	71.318	-354.871	18.855
1000	51.882	109.823	74.901	-356.100	16.450
1100	52.347	114.790	78.305	-357.385	14.472
1200	52.802	119.365	81.538	-358.726	12.824
1300	53.252	123.609	84.613	-360.122	11.429
1400	53.681	127.571	87.542	-361.573	10.275
1500	54.073	131.288	90.335	-363.077	9.323
1600	54.476	134.791	93.005	-364.634	8.539
1700	54.910	138.106	95.562	-366.244	7.893
1800	55.312	141.256	98.014	-367.907	7.365
1900	55.687	144.256	100.369	-369.624	6.843
2000	56.024	147.120	102.636	-371.396	6.325
2100	56.468	149.864	104.820	-373.224	5.811
2200	56.902	152.501	106.927	-375.108	5.302
2300	57.326	155.039	108.964	-377.048	4.798
2400	57.739	157.488	110.935	-379.044	4.300
2500	58.131	159.853	112.845	-381.096	3.808
2600	58.534	162.141	114.697	-383.204	3.332
2700	58.953	164.358	116.496	-385.368	2.871
2800	59.371	166.509	118.244	-387.588	2.424
2900	59.789	168.600	119.944	-389.864	1.991
3000	60.208	170.634	121.600	-392.196	1.572

PREVIOUS: December 1971

CURRENT: September 1977

Magnesium Sulfide (MgS)

Mg₃S₄(cr)

Magnesium Sulfide (MgS)

IDEAL GAS

Magnesium Sulfide (MgS)

Mg₂S₃(g)

$S^{\circ}(298.15\text{ K}) = 225.483 \pm 4.2\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $\Delta H^{\circ}(0\text{ K}) = [145.39 \pm 66.9]\text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta H^{\circ}(298.15\text{ K}) = [145.23 \pm 66.9]\text{ kJ}\cdot\text{mol}^{-1}$

State	ϵ_{ν} , cm^{-1}	g_{ν}	ω_{ν} , cm^{-1}	$\omega_{\nu}x_{\nu}$, cm^{-1}	B_{ν} , cm^{-1}	α_{ν} , cm^{-1}	r_{ν} , Å	Source
X ¹ Σ ⁺	0.0	1	526.47	2.681	0.26570	0.00174	2.1425	1
II	[2000]	6	[430]	[2.2]	[0.237]	[0.0015]	[2.27]	2
II	[3000]	2	[430]	[2.2]	[0.237]	[0.0015]	[2.27]	3
X ² Σ ⁺	[17000]	3	[493.20]	[2.313]	[0.2530]	[0.00153]	[2.1956]	1, 2
A ¹ Σ ⁺	23036.98	1	495.20	2.313	0.2530	0.00153	2.1956	1

Enthalpy of Formation

Colin *et al.*¹ searched unsuccessfully for gaseous MgS in a Knudsen effusion mass-spectrometric experiment. They set the upper limit $D_0^{\circ}(\text{MgS}, g) = 55\text{ kcal}\cdot\text{mol}^{-1}$. There are no other equilibrium or positive mass spectrometric data involving MgS(g); consequently $D_0^{\circ}(\text{MgS}, g)$ must be estimated. The Birge-Sponer extrapolation is of little utility in this case. Gaydon² has gone into great detail concerning the problems inherent in linear-Birge-Sponer extrapolations (LBX) on the oxides and sulfides of the alkaline earths. The normal LBX yields $D_0^{\circ}(\text{MgS}, g) = 73\text{ kcal}\cdot\text{mol}^{-1}$. When adjusted for ionic character with the Hildenbrand correction,³ $D_0^{\circ}(\text{MgS}, g) = 65\text{ kcal}\cdot\text{mol}^{-1}$. The ground state of MgS cannot dissociate into ground state atoms. After correcting for the excited atomic products, $D_0^{\circ}(\text{MgS}, g) = 42\text{ kcal}\cdot\text{mol}^{-1}$. A more reliable method of estimation is that of Haug and Margrave⁴ based on the observation that the ratio $D_{\text{MgS}}/D_{\text{MgO}}$ is very similar for elements within a given group. Based on data involving known bond energies and force constants of the gaseous diatomic oxides and sulfides, we calculate $D_0^{\circ}(\text{MgS}, g) = 78 \pm 10\text{ kcal}\cdot\text{mol}^{-1}$. Dissociation energies of the alkaline earth monoxides were taken from Srivastava,⁵ dissociation energies for the alkaline earth sulfides were taken from JANAF Thermochemical Tables,⁶ and force constants were calculated from spectroscopic data of Barrow and Cousins.⁷ Further comparisons of vapor pressures and enthalpies of sublimation for the other alkaline earth oxides and sulfides⁸ suggest lower values of $D_0^{\circ}(\text{MgS}, g)$ than the Haug and Margrave method leads to. We adopt $D_0^{\circ}(\text{MgS}, g) \leq 66 \pm 16\text{ kcal}\cdot\text{mol}^{-1}$. Using auxiliary JANAF data,⁶ we calculate $\Delta H^{\circ}(\text{MgS}, g, 298.15\text{ K}) = 34.71 \pm 16\text{ kcal}\cdot\text{mol}^{-1}$.

Heat Capacity and Entropy

The spectroscopic constants of the observed states, taken from Marcano and Barrow⁹ for the isotopic species Mg²⁴S³², are corrected to account for the natural abundances of the elements. Other low-lying electronic states and their vibrational-rotational constants are estimated in isoelectronic groups by analogy with MgO⁹ and from trends observed in the known states of the other alkaline-earth oxides and sulfides.⁶ Uncertainty in the energy and molecular constants for the estimated states may contribute significantly, perhaps as much as 1.0 cal·K⁻¹·mol⁻¹ to the entropy at 298.15 K.

The ground state of gaseous MgS is taken as ¹Σ⁺. There should be low-lying triplet states. A ¹Π state is predicted for MgS at 3000 cm⁻¹ based on experimentally observed ¹Π states for MgO,⁹ BeO,¹⁰ and BeS.¹⁰ The corresponding triplet, ³Π₁, is assumed to lie 1000 cm⁻¹ lower in energy based on trends in the triplet-singlet splitting observed by Field¹¹ for the alkaline-earth oxides. Similar trends in the triplet-singlet splitting of the isoelectronic Σ states are used to place the ³Σ⁺ state 6000 cm⁻¹ below the experimentally observed⁶ A¹Σ⁺ state. By analogy with MgO⁹ we do not feel that a Δ state exists below 25000 cm⁻¹. The thermodynamic functions are calculated using first-order anharmonic corrections to Q_v and Q_r in the partition function $Q = Q_{\nu} \sum Q_{\nu} \cdot g_{\nu} \cdot \exp(-\epsilon_{\nu}/T)$.

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T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p ^o = 0.1 MPa		log K _t
	C _p ^o	S ^o - (C _p ^o - H ^o (T _r))/T _r	H ^o - H ^o (T _r)	ΔG ^o	
	J·K ⁻¹ ·mol ⁻¹	J·K ⁻¹ ·mol ⁻¹	kJ·mol ⁻¹	kJ·mol ⁻¹	
0	0	INFINITE	-9.245	145.392	INFINITE
100	29.371	191.105	-6.332	146.973	130.625
200	32.039	212.204	-3.273	146.383	79.939
250	33.380	219.500	-1.636	145.829	105.090
298.15	34.599	225.483	0	145.227	97.297
300	34.648	225.697	0.064	145.203	16.889
350	36.111	231.144	1.832	144.542	89.018
400	37.572	236.082	3.682	141.668	10.606
450	40.277	240.684	5.636	140.377	8.559
500	42.922	245.062	7.715	139.107	6.639
600	48.397	253.377	12.284	137.324	52.038
700	53.741	261.186	17.356	136.177	2.830
800	55.100	268.406	22.765	135.386	-1.563
900	55.994	274.940	28.313	134.559	-0.646
1000	54.817	280.766	33.842	133.575	-0.209
1100	53.380	285.926	39.255	132.486	0.140
1200	51.717	290.500	44.510	131.274	0.431
1300	50.079	294.574	49.599	129.951	-9.896
1400	48.585	298.230	54.531	128.527	0.676
1500	47.278	301.536	59.323	127.007	0.768
1600	46.161	304.555	63.993	125.492	0.633
1700	45.217	307.320	68.560	123.986	0.516
1800	44.426	309.881	73.042	122.498	0.414
1900	43.765	312.265	77.450	121.027	0.325
2000	43.213	314.496	81.798	119.576	0.245
2100	42.752	316.592	86.096	118.144	0.174
2200	42.368	318.572	90.351	116.728	0.110
2300	42.048	320.448	94.572	115.335	0.052
2400	41.781	322.232	98.763	113.964	-0.001
2500	41.559	323.933	102.929	112.618	-0.049
2600	41.375	325.559	107.076	111.298	-0.094
2700	41.225	327.118	111.205	109.998	-0.135
2800	41.102	328.615	115.321	108.721	-0.173
2900	41.003	330.055	119.426	107.466	-0.208
3000	40.925	331.444	123.523	106.232	-0.241
3100	40.865	332.785	127.612	105.017	-0.272
3200	40.820	334.081	131.696	103.822	-0.301
3300	40.790	335.337	135.776	102.646	-0.328
3400	40.772	336.554	139.854	101.489	-0.353
3500	40.764	337.736	143.931	100.352	-0.378
3600	40.766	338.883	148.008	99.235	-0.400
3700	40.776	340.002	152.085	98.138	-0.422
3800	40.793	341.089	156.163	97.061	-0.442
3900	40.817	342.149	160.243	96.004	-0.460
4000	40.847	343.183	164.327	94.967	-0.478
4100	40.882	344.192	168.413	93.949	-0.498
4200	40.921	345.178	172.503	92.952	-0.515
4300	40.965	346.141	176.597	91.975	-0.531
4400	41.012	347.083	180.696	91.018	-0.547
4500	41.062	348.005	184.800	90.081	-0.562
4600	41.115	348.909	188.909	89.164	-0.576
4700	41.170	349.793	193.023	88.267	-0.590
4800	41.228	350.661	197.143	87.390	-0.604
4900	41.287	351.511	201.269	86.533	-0.617
5000	41.348	352.346	205.400	85.696	-0.630
5100	41.410	353.166	209.538	84.879	-0.642
5200	41.473	353.970	213.682	84.082	-0.654
5300	41.537	354.761	217.833	83.305	-0.667
5400	41.602	355.538	221.990	82.548	-0.677
5500	41.668	356.302	226.153	81.811	-0.688
5600	41.734	357.053	230.323	81.094	-0.698
5700	41.801	357.792	234.507	80.407	-0.709
5800	41.868	358.520	238.695	79.749	-0.719
5900	41.935	359.236	242.874	79.122	-0.729
6000	42.002	359.942	247.070	78.526	-0.739

PREVIOUS: September 1977 (1 atm)

CURRENT: September 1977 (1 bar)

Magnesium Sulfide (MgS)

Mg₂S₃(g)

Mg₂(g)

Mg₂ Magnesium (Mg₂)

IDEAL GAS

Magnesium (Mg₂)

$D_0^0 = 4.84 \pm 0.01 \text{ kJ}\cdot\text{mol}^{-1}$ (natural abundance)
 $S^0(298.15 \text{ K}) = 240.19 \pm 0.50 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $\Delta H_f^0(298.15 \text{ K}) = 288.16 \pm 0.80 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta H_f^0(298.15 \text{ K}) = 287.63 \pm 0.80 \text{ kJ}\cdot\text{mol}^{-1}$

State	T_c	D^0	ω_e	$\omega_e x_e$	B_e	$10^4 D_e$	$r_e, \text{ \AA}$	References
$^1\Sigma_g^+$	0	404	51.121	1.6448 ^a	0.092866	1.2166 ^b	3.8905	1
$^3\Pi_g$	[15645]	[21740]	[220.1]	[1.95]	[0.171]	[1.89]	[2.91]	4 ^d
$^3\Sigma_g^-$	[16773]	[21740]	[184.2]	[1.67]	[0.145]	[0.359]	[3.18]	4 ^d
$^1\Pi_g$	[20267]	[34941]	[263.1]	[1.17]	[0.181]	[1.15]	[2.91]	4 ^d

(a) $+1.6244 \times 10^{-2} (v + 1/2)^3 - 6.106 \times 10^{-4} (v + 1/2)^4$
 (b) $+1.0679 \times 10^{-4} (v + 1/2)^2 - 9.6831 \times 10^{-6} (v + 1/2)^3$
 (c) $-3.0768 \times 10^{-4} (v + 1/2) + 2.1344 \times 10^{-8} (v + 1/2)^2$
 (d) These values are estimated based on the theoretical potential curves of Stevens and Krauss.⁴

Enthalpy of Formation

The ground state dissociation energy for 2Mg_2 was determined by Li and Stwalley² to be $404.1 \pm 0.5 \text{ cm}^{-1}$. This value was corrected to natural abundance Mg_2 with the result $D_0^0 = 404.3 \text{ cm}^{-1}$. Using this value and the recommended value for $\Delta H_f^0(Mg, g, 0) = 146,499 \text{ kJ}\cdot\text{mol}^{-1}$ from CODATA,¹³ we calculate the adopted value of $\Delta H_f^0(Mg_2, g, 0) = 288.16 \text{ kJ}\cdot\text{mol}^{-1}$. Our adopted D^0 is in essential agreement with the value adopted by Brewer² and by Wagman *et al.*³ It should be noted that a value of $D_0^0 = 11.3 \pm 4.1 \text{ kJ}\cdot\text{mol}^{-1}$ was determined by a mass spectrometric study of Wu, Ihle and Gingerich.⁷ In light of the spectroscopic evidence, this value appears to be too large.

Heat Capacity and Entropy

The thermal functions are calculated using a direct summation technique analogous to the alkali dimers and diatomic halogens. Included in the calculation are the ground state and the three lowest excited states. Spectroscopic constants for the $^1\Sigma_g^+$ ground state are taken from an experimental study from Balfour and Douglas.¹ No known spectroscopic data exists for the three lowest excited electronic states of $Mg_2(g)$. In order to generate the spectroscopic constants of these states, a Morse potential was least squares fit to the calculated potential curves of Stevens and Krauss,⁴ an ab initio investigation which included configuration interaction. Although this procedure for estimating the spectroscopic data results in substantial uncertainty in the generated constants, the inclusion of the excited states results in thermal functions which are more realistic at temperatures greater than 1000 K. The large maximum in the heat capacity at 5000 K, for example, would not be present if the excited states were not included. Also, it should be noted that $Mg_2(g)$ is an example of a molecule where the traditional integration methods of calculating the thermal functions fail due to the shallow ground state.

The rotational levels are extrapolated to high J values according to the method of Khachkuruzov⁹ who proposed a simpler form of Woolley's method.⁶ For the ground state only, we included the so-called quasi-bound rotational levels above the dissociation limit.⁹ The values used for J_{min} and v_{max} are 93 and 17, respectively, as determined by¹ Separate calculations were performed for each of the six isotopic dimeric species (made up from the three atomic isotopes ^{24}Mg , ^{25}Mg , ^{26}Mg) by adjusting the spectroscopic constants of ^{24}Mg using a standard reduced mass scaling routine.¹⁰ The results were combined according to the natural abundance of the atoms, ^{24}Mg : 78.99%, ^{25}Mg : 10.00%, ^{26}Mg : 11.01%.¹¹ Splitting of the rotational levels in the $^1\Pi_g$ and $^3\Sigma_g^-$ states was taken into account only insofar as the degeneracy of these states were increased accordingly. The adopted value of $S^0(298.15 \text{ K})$ is $0.64 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$, smaller than that adopted by⁸

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T/K	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K _r
	C _p ^o	S° - [C _p ° - H _f °(T)]/T	H _f ° - H _f °(T)	ΔG°	
0	0.000	0.000	INFINITE	INFINITE	INFINITE
100	38.343	206.636	288.158	288.158	-141.949
200	28.193	229.790	290.515	271.572	-66.099
250	23.571	235.789	240.594	244.015	-50.984
298.15	24.293	240.186	235.495	235.495	-41.238
300	24.250	240.337	235.172	235.172	-40.947
350	23.430	244.001	236.242	236.242	-33.809
400	22.742	247.076	238.420	238.420	-28.482
450	22.129	249.726	240.843	240.843	-24.360
500	21.634	252.066	243.528	243.528	-21.081
600	21.149	256.046	247.711	247.711	-16.203
700	20.748	259.365	252.464	252.464	-12.762
800	20.408	262.214	257.692	257.692	-10.216
900	20.166	264.713	263.206	263.206	-8.265
1000	20.093	266.939	268.947	268.947	-6.803
1100	20.039	268.947	273.103	273.103	-5.649
1200	20.999	270.776	276.691	276.691	-4.707
1300	20.967	272.455	280.628	280.628	-3.925
1400	20.944	274.008	284.957	284.957	-3.306
1500	20.927	275.452	289.721	289.721	-2.817
1600	20.919	276.803	294.876	294.876	-2.430
1700	20.923	278.071	300.471	300.471	-2.133
1800	20.946	279.267	306.556	306.556	-1.904
1900	20.998	280.401	313.182	313.182	-1.735
2000	21.094	281.480	320.326	320.326	-1.618
2100	21.253	282.513	327.971	327.971	-1.540
2200	21.497	283.507	336.116	336.116	-1.499
2300	21.833	284.470	344.761	344.761	-1.483
2400	22.351	285.410	353.906	353.906	-1.487
2500	23.024	286.336	363.551	363.551	-1.503
2600	23.904	287.255	373.696	373.696	-1.529
2700	25.023	288.172	384.341	384.341	-1.564
2800	26.412	289.112	395.486	395.486	-1.608
2900	28.096	290.067	407.131	407.131	-1.660
3000	30.094	291.052	419.276	419.276	-1.719
3100	32.417	292.076	431.921	431.921	-1.784
3200	35.067	293.146	445.066	445.066	-1.854
3300	38.032	294.270	458.711	458.711	-1.928
3400	41.290	295.453	472.856	472.856	-2.006
3500	44.885	296.700	487.501	487.501	-2.088
3600	48.826	298.014	502.646	502.646	-2.174
3700	53.133	299.396	518.291	518.291	-2.264
3800	56.336	300.845	534.436	534.436	-2.358
3900	60.277	302.360	551.081	551.081	-2.456
4000	64.134	303.935	568.226	568.226	-2.558
4100	67.825	305.564	585.871	585.871	-2.664
4200	71.274	307.240	604.016	604.016	-2.774
4300	74.410	308.955	622.661	622.661	-2.888
4400	77.176	310.698	641.806	641.806	-2.998
4500	79.525	312.460	661.451	661.451	-3.104
4600	81.426	314.229	681.596	681.596	-3.206
4700	82.864	315.996	702.241	702.241	-3.304
4800	83.838	317.752	723.386	723.386	-3.398
4900	84.358	319.487	745.031	745.031	-3.488
5000	84.450	321.193	767.176	767.176	-3.574
5100	84.145	322.863	790.821	790.821	-3.656
5200	83.481	324.491	815.966	815.966	-3.734
5300	82.502	326.076	842.611	842.611	-3.808
5400	81.254	327.603	870.756	870.756	-3.878
5500	79.780	329.081	900.401	900.401	-3.944
5600	78.126	330.504	931.546	931.546	-4.006
5700	76.331	331.871	964.191	964.191	-4.064
5800	74.435	333.182	1000.336	1000.336	-4.118
5900	72.470	334.438	1040.981	1040.981	-4.168
6000	70.466	335.639	1086.126	1086.126	-4.214

PREVIOUS: December 1974 (1 atm)

CURRENT: September 1983 (1 bar)

Mg₂(g)

Magnesium (Mg₂)

Mg₂O₃Si₁(cr)

Magnesium Silicate (Mg₂SiO₄)

M_r = 140.6931

CRYSTAL

Magnesium Silicate (Mg₂SiO₄)

Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		
T/K	C _p ^o / J·K ⁻¹ ·mol ⁻¹	H° - H°(T _r) / kJ·mol ⁻¹	ΔG° / kJ·mol ⁻¹	log K _r
0	0	0	-2163.634	INFINITE
100	32.317	-17.280	-2169.994	1114.924
200	86.144	-10.180	-2096.757	547.617
298.15	118.688	0	-2057.879	360.532
300	119.148	0.220	-2057.131	358.180
400	137.557	13.141	-2017.207	263.410
500	148.695	27.491	-1977.171	206.554
600	156.431	42.767	-1937.386	168.664
700	162.310	58.715	-1897.782	141.615
800	167.063	75.191	-1858.375	121.339
900	171.088	92.104	-1819.128	105.579
1000	174.607	109.392	-1778.598	92.904
1100	177.770	127.013	-1737.746	82.519
1200	180.665	144.936	-1697.000	74.868
1300	183.360	163.139	-1656.367	68.554
1400	185.895	181.602	-1615.916	60.052
1500	188.369	200.314	-1575.560	53.995
1600	190.619	219.261	-1535.326	48.706
1700	192.845	238.434	-1495.288	44.034
1800	195.008	257.828	-1455.404	39.816
1900	197.108	277.434	-1415.615	36.049
2000	199.163	297.248	-1375.974	32.667
2100	201.175	317.264	-1336.426	29.614
2171.000	202.673	331.600	-1296.926	---
2200	203.154	337.487	-1257.426	26.845
2300	205.100	357.900	-1170.953	24.322
2400	207.020	378.506	-1084.534	22.015
2500	208.915	399.303	-998.166	19.899
2600	210.790	420.289	-911.854	17.950
2700	212.648	441.461	-825.504	16.150
2800	214.490	462.818	-739.116	14.483
2900	216.315	484.358	-652.692	12.935
3000	218.124	506.080	-566.232	11.495

S°(298.15 K) = 95.14 ± 0.8 J·K⁻¹·mol⁻¹
 T_m = 2171 ± 11 K
 ΔH_f°(0 K) = -2163.63 ± 4.2 kJ·mol⁻¹
 ΔH_f°(298.15 K) = -2176.94 ± 4.2 kJ·mol⁻¹
 Δ_{hyd}H° = [71.128 ± 20.9] kJ·mol⁻¹

Enthalpy of Formation

Torgeson *et al.*¹ have reported a ΔH_f°(298.15 K) = -15.1 ± 0.2 kcal·mol⁻¹ for reaction (a). They used an HF solution calorimeter and measured the enthalpies of solution of each component. We derive ΔH_f°(Mg₂SiO₄, cr, 298.15 K) = -520.30 ± 1.0 kcal·mol⁻¹ using the ΔH_f°(298.15 K) of MgO(cr) and SiO₂(cr, low quartz) from JANAF tables.

Kapustinski *et al.*² used the same method but measured only ΔH_f°(298.15 K) of H₂SiF₆(aq) from source 3 and the ΔH_f°(298.15 K) of H₂O(l) and HF(aq) from source 4.

Reesman *et al.*³ calculated a ΔG°(298.15 K) = 42.46 kcal·mol⁻¹ for reaction (c) using aqueous solubility data. We use the ΔG°(298.15 K) of H₂O(l) and OH⁻(aq) from source 4, ΔG°(298.15 K) of H₂SiO₄(aq) from source 3 and ΔG°(298.15 K) of Mg²⁺(aq) from source 6 and we obtain a ΔG°(Mg₂SiO₄, cr, 298.15 K) = -498.764 kcal·mol⁻¹. We derive a ΔH_f°(Mg₂SiO₄, cr, 298.15 K) = -524.848 kcal·mol⁻¹ using the above ΔG°(298.15 K) of Mg₂SiO₄(cr) and the entropies of Mg(cr), Si(cr) and O₂(g) from the JANAF tables.

The adopted value is from the work of Torgeson *et al.*¹ which is considered to be the most reliable since it relates directly to the oxides. The other reported values are less accurate and involve uncertainties in the auxiliary data used to derive the heat of formation.

Source	Method	Reaction	ΔH _f °(298.15 K) / kcal·mol ⁻¹	ΔG°(298.15 K) / kcal·mol ⁻¹	ΔH _f °(298.15 K) / kcal·mol ⁻¹
1	hydrofluoric acid solution calorimeter	(a) 2 MgO(cr) + SiO ₂ (cr) = Mg ₂ SiO ₄ (cr)	-15.10 ± 0.2	-520.3	
2	hydrofluoric acid solution calorimeter	(b) Mg ₂ SiO ₄ (cr) + 10 HF(aq, 4.44 H ₂ O) = 2 MgF ₂ (cr) + H ₂ SiF ₆ (714 HF(aq) + 322 OH ₂ O) + 4 H ₂ O(l)	95.0 ± 0.47	-522.27	
3	aqueous solubility	(c) Mg ₂ SiO ₄ (cr) + 4 H ₂ O(l) = 2 Mg ²⁺ (aq) + H ₂ SiO ₄ (aq) + 4 OH ⁻ (aq)	42.46	-524.848	

Heat Capacity and Entropy

Low temperature heat capacities are from the data (53–295 K) of Kelley.⁷ High temperature enthalpies have been measured (398–1808 K) by Orr.⁸ High temperature heat capacities are derived from the enthalpies by a fitting technique which constrains the curve to join smoothly with the low temperature values. The entropy is based on S°(50 K) = 0.60 cal·K⁻¹·mol⁻¹.

Fusion Data

T_m is obtained from Davis *et al.*⁹ Δ_{hyd}H° is estimated from MacGregor's¹⁰ phase diagrams of the Mg₂SiO₄-TiO₂ system. The phase diagrams were determined at 10 and 20 kbars pressure.

References

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PREVIOUS: September 1964

CURRENT: December 1967

Magnesium Silicate (Mg₂SiO₄)

Mg₂O₃Si₁(cr)

Magnesium Silicate (Mg₂SiO₄)

LIQUID

M_r = 140.6931 Magnesium Silicate (Mg₂SiO₄)

Mg₂O₂Si₁(l)

S°(298.15 K) = [123.044] J·K⁻¹·mol⁻¹
 T_{fus} = 2171 ± 11 K

Δ_{cr}H°(298.15 K) = [-2113.88 ± 20.9] kJ·mol⁻¹
 Δ_{liq}H° = [71.128 ± 20.9] kJ·mol⁻¹

Enthalpy of Formation

Δ_{cr}H°(Mg₂SiO₄, l, 298.15 K) is calculated from Δ_{cr}H°(Mg₂SiO₄, cr, 298.15 K) by adding Δ_{liq}H° and the difference in enthalpy, H°(2171 K) - H°(298.15 K), between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 1400 K. Below 1400 K the heat capacity is obtained from the heat capacity of the crystal. Above 1400 K the heat capacity is assumed constant and estimated as 49 cal·K⁻¹·mol⁻¹ or 7 cal·K⁻¹·g-atom⁻¹ or 7 cal·K⁻¹·mol⁻¹ and estimated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

T/K	C _p ^o	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
		S° - [G° - HF(T)]/T	H° - H°(T _r)	Δ _{cr} H°	Δ _{liq} H°	
0			0.			
100						
200						
298.15	118.688	123.044	123.044	0.	-2113.878	350.942
300	119.148	123.780	123.046	0.220	-2113.895	348.658
400	137.357	160.824	127.972	13.141	-2114.149	256.633
500	148.695	192.798	137.817	21.491	-2113.528	201.424
600	156.431	220.628	149.351	42.767	-2112.482	164.632
700	162.310	245.201	161.323	58.715	-2111.235	138.367
800	167.063	267.195	173.206	75.191	-2109.918	118.680
900	171.088	287.110	184.773	92.104	-2108.615	103.377
1000	174.607	305.322	195.930	109.392	-2124.574	91.068
1100	177.770	322.114	206.648	127.013	-2123.489	80.982
1200	180.665	337.708	216.928	144.936	-2122.224	72.581
1300	183.360	352.276	226.785	163.139	-2120.789	65.478
1400	185.895	365.958	236.242	181.603	-2119.015	59.157
1400.000	185.895	365.958	236.242	181.603	GLASS <---> LIQUID	
1400.000	205.016	365.958	236.242	181.603	TRANSITION	
1500	205.016	380.103	245.367	202.104	-2367.777	53.259
1600	205.016	393.334	254.206	222.606	-2361.633	48.112
1700	205.016	405.763	262.759	243.108	-2405.758	43.569
1800	205.016	417.482	271.032	263.609	-2399.565	39.468
1900	205.016	428.567	279.035	284.111	-2393.419	35.807
2000	205.016	439.082	286.776	304.612	-2387.319	32.572
2100	205.016	449.085	294.269	325.114	-2381.266	29.556
2171.000	205.016	455.902	299.444	339.670	---	---
2200	205.016	458.623	301.524	345.616	-2375.259	26.867
2300	205.016	467.736	308.555	366.117	-2369.298	24.418
2400	205.016	476.461	315.370	386.619	-2363.384	22.179
2500	205.016	484.830	321.982	407.120	-2357.515	20.124
2600	205.016	492.871	328.401	427.622	-2351.693	18.232
2700	205.016	500.609	334.637	448.124	-2345.917	16.484
2800	205.016	508.065	340.699	468.625	-2340.189	14.865
2900	205.016	515.259	346.595	489.127	-2334.508	13.362
3000	205.016	522.209	352.333	509.628	-2328.877	11.962
3100	205.016	528.932	357.922	530.130	-2323.296	10.655
3200	205.016	535.441	363.368	550.632	-2317.767	9.433
3300	205.016	541.749	368.679	571.133	-2312.291	8.288
3400	205.016	547.870	373.860	591.635	-2306.872	7.213
3500	205.016	553.813	378.917	612.136	-2301.510	6.201
3600	205.016	559.588	383.855	632.638	-2296.202	5.297
3700	205.016	565.203	388.681	653.140	-2290.947	4.447
3800	205.016	570.673	393.399	673.641	-2285.743	3.654
3900	205.016	575.998	398.013	694.143	-2280.586	2.914
4000	205.016	581.189	402.578	714.644	-2275.476	2.223

PREVIOUS: September 1964

CURRENT: December 1967

Magnesium Silicate (Mg₂SiO₄)

Mg₂O₂Si₁(l)

Mg₂O₄Si₁(cr,l)

M_r = 140.6931 Magnesium Silicate (Mg₂SiO₄)

CRYSTAL-LIQUID

Magnesium Silicate (Mg₂SiO₄)

0 to 2171 K crystal
above 2171 K liquid
Refer to the individual tables for details.

T/K	C _p ^a	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
		S° - [G° - H°(T _r)]/T	H° - H°(T _r)/T	Δ _r H°	Δ _r G°	
0	0	INFINITE	-17.280	-2163.634	-2163.634	INFINITE
100	32.317	14.050	-16.280	-2134.453	-2134.453	1114.924
200	86.144	54.162	-10.180	-2096.757	-2096.757	547.617
298.15	118.688	95.140	0	-2176.935	-2057.879	360.532
300	119.148	95.876	0.220	-2176.953	-2057.141	358.180
400	157.557	132.920	13.141	-2177.207	-2017.151	263.410
500	148.695	164.894	27.491	-2176.585	-1977.171	206.554
600	156.431	192.724	42.767	-2175.539	-1937.382	168.664
700	162.310	217.297	58.715	-2174.292	-1897.786	141.615
800	167.063	239.291	75.191	-2172.975	-1858.375	121.339
900	171.088	259.206	92.104	-2171.673	-1819.128	105.579
1000	174.607	277.418	108.026	-2170.392	-1778.598	92.904
1100	177.770	294.210	127.013	-2169.147	-1737.746	82.519
1200	180.665	309.804	144.936	-2167.931	-1697.000	73.868
1300	183.360	324.372	163.139	-2166.747	-1656.367	66.554
1400	185.895	338.054	181.602	-2165.593	-1616.516	60.052
1500	188.309	350.962	200.314	-2164.466	-1578.560	53.995
1600	190.619	363.190	219.261	-2163.366	-1542.904	48.706
1700	192.845	374.813	238.434	-2162.291	-1509.093	44.034
1800	195.008	385.897	257.828	-2161.240	-1477.040	39.816
1900	197.108	396.497	277.434	-2160.213	-1446.573	36.049
2000	199.163	406.660	297.248	-2159.210	-1417.687	32.667
2100	201.175	416.426	317.264	-2158.231	-1390.375	29.614
2171.000	202.673	423.139	331.600	-2157.275	-1364.558	26.867
2171.000	205.016	455.902	402.728	-2156.333	-1340.186	24.418
2200	205.016	458.623	408.673	-2155.403	-1317.186	22.179
2300	205.016	467.736	429.175	-2154.484	-1295.047	20.124
2400	205.016	476.461	449.616	-2153.575	-1273.751	18.232
2500	205.016	484.830	470.178	-2152.675	-1253.304	16.484
2600	205.016	492.871	490.680	-2151.783	-1233.807	14.865
2700	205.016	500.609	511.282	-2150.899	-1215.260	13.362
2800	205.016	508.065	531.683	-2150.023	-1197.573	11.962
2900	205.016	515.259	552.850	-2149.154	-1180.646	10.655
3000	205.016	522.209	573.686	-2148.291	-1164.479	9.433
3100	205.016	528.932	593.188	-2147.434	-1148.972	8.288
3200	205.016	535.441	613.689	-2146.583	-1134.124	7.213
3300	205.016	541.749	634.191	-2145.737	-1119.933	6.201
3400	205.016	547.870	654.692	-2144.895	-1106.400	5.097
3500	205.016	553.813	675.194	-2144.057	-1093.525	4.027
3600	205.016	559.588	695.696	-2143.223	-1081.307	3.054
3700	205.016	565.203	716.197	-2142.393	-1069.744	2.174
3800	205.016	570.673	736.699	-2141.566	-1058.837	1.384
3900	205.016	575.998	757.200	-2140.742	-1048.584	0.663
4000	205.016	581.189	777.702	-2140.000	-1038.986	0.000

PREVIOUS

CURRENT: December, 1967

Magnesium Silicate (Mg₂SiO₄)

Mg₂O₄Si₁(cr,l)

Mg₂O₄Ti₁(cr)

Magnesium Titanium Oxide (Mg₂TiO₄)

M_r = 160.4876

CRYSTAL

Magnesium Titanium Oxide (Mg₂TiO₄)

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa	
	C _p ^o	S° - [C _p ° - F(T _r)]/T	H° - H(T _r)	ΔG°
0	0	INFINITE	-18.836	-2151.027
100	34.639	06.740	-17.753	-2127.882
200	94.320	70.337	-11.113	-2085.881
298.15	128.574	115.102	0	-2047.719
300	129.026	115.899	0.238	-2046.995
400	146.283	120.405	14.093	-2007.859
500	156.410	129.441	29.260	-1968.875
600	163.686	143.161	45.280	-1930.176
700	169.882	155.811	61.852	-1891.618
800	174.707	168.317	79.171	-1853.319
900	179.360	180.509	96.877	-1815.267
1000	183.686	192.243	115.032	-1775.953
1100	187.778	203.515	133.607	-1736.349
1200	191.690	214.332	152.581	-1696.756
1300	195.456	224.714	171.940	-1657.101
1400	199.091	234.689	191.668	-1617.300
1500	202.614	244.282	211.754	-1577.467
1600	206.041	253.520	232.188	-1496.007
1700	209.367	262.429	252.959	-1438.908
1800	212.610	271.033	274.058	-1382.158
1900	215.765	279.353	295.478	-1325.745
2000	218.840	287.410	317.209	-1269.205
2013.000	219.233	288.438	320.056	---
2100	221.831	295.220	339.243	-1212.657
2200	224.752	302.800	361.573	-1156.379
2300	227.593	310.165	384.191	-1100.373
2400	230.358	317.329	407.089	-1044.637
2500	233.049	324.304	430.260	-989.168
2600	235.668	331.101	453.696	-933.964
2700	238.212	337.730	477.391	-879.024
2800	240.685	344.201	501.336	-824.346
2900	243.086	350.522	525.525	-769.929
3000	245.417	356.701	549.951	-715.767

Δ_rH°(0 K) = -2151.03 ± 6.3 kJ·mol⁻¹
 Δ_rH°(298.15 K) = -2164.38 ± 6.3 kJ·mol⁻¹
 Δ_{sub}F° = [129.704] kJ·mol⁻¹

Enthalpy of Formation

The enthalpy of formation is calculated from Δ_rF°(298.15 K) = -4.1 ± 0.25 kcal·mol⁻¹ for the reaction 2 MgO(cr) + TiO₂(rutile) → Mg₂TiO₄(cr) measured by Kelley,¹ using a solution calorimetric method. The uncertainty of ±1.5 kcal·mol⁻¹ assigned to the enthalpy of formation is due primarily to TiO₂(rutile)

Heat Capacity and Entropy

Low temperature heat capacities are from the data (52–296 K) of Todd.² High temperature heat capacities are derived from the enthalpies by a fitting technique which constrains the curve to join smoothly with the low temperature values.

The entropy is based on S°(51 K) = 0.66 + 2.75 = 3.41 cal·K⁻¹·mol⁻¹, where the first term is a lattice contribution and the second term is a zero-point entropy of 2Rln2 corresponding to random distribution of Ti and Mg on the octahedral sites of the spinel lattice. The adopted value is S°(298.15 K) = 27.51 ± 1.5 cal·K⁻¹·mol⁻¹ instead of 24.76 ± 0.15 cal·K⁻¹·mol⁻¹ as given by Todd.

Barth³ showed from intensities of the x-ray diffraction lines that Mg₂TiO₄ is a spinel of the inverse (or variate) class. Thus, half of the Mg ions occupy the tetrahedral interstices in the oxygen lattice, while the remaining Mg ions and the Ti ions are (presumably) randomly located in the octahedral interstices. This conclusion was confirmed by Romeijn.⁴

King and Kelley⁶ suggested that the degree of structural randomness is not established and that it may vary with the sample of Mg₂TiO₄; thus, they recommended an intermediate value of Rln2 for the zero-point entropy. In a previous review, however, Kelley¹ used the theoretical value of 2Rln2 in order to make Mg₂TiO₄ stable relative to MgTiO₃ at high temperatures. We choose to adopt 2Rln2, although the evidence is not conclusive. Recent studies of solid state reactions by Bausch and Werner⁷ indicate that Δ_rG° is negative for Mg-TiO₃(cr) + MgO(cr) → Mg₂TiO₄(cr) at temperatures of 1673 K and above. Both Rln2 and 2Rln2 are consistent with this evidence.

Fusion Data

Refer to the liquid table for details.

References

1. K. K. Kelley, S. S. Todd and E. G. King, U. S. Bur. Mines RI 5059, (1954).
2. S. Todd, J. Amer. Chem. Soc. 74, 4669 (1952).
3. R. L. Orr and J. P. Coughlin, J. Amer. Chem. Soc. 74, 3186 (1952).
4. T. F. W. Barth and E. Postnjak, Z. Krist. 82, 325 (1932).
5. E. G. King and K. K. Kelley, U. S. Bur. Mines RI 5502, (1959).
6. H. J. Bausch and I. Werner, Silikat Tech. 14, 203 (1963).

PREVIOUS: June 1961

CURRENT: June 1967

Magnesium Titanium Oxide (Mg₂TiO₄)

Mg₂O₄Ti₁(cr)

Mg₂O₄Ti₂(l)

Mg₂O₄Ti₂(l)

M_r = 160.4876

LIQUID

Magnesium Titanium Oxide (Mg₂TiO₄)

$S^\circ(298.15 \text{ K}) = [172.412] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$
 $T_{\text{fus}} = 2013 \pm 20 \text{ K}$
 $\Delta_r H^\circ(298.15 \text{ K}) = [-2046.33 \pm 6.3] \text{ kJ} \cdot \text{mol}^{-1}$
 $\Delta_{\text{fus}} H^\circ = [129.704] \text{ kJ} \cdot \text{mol}^{-1}$

Enthalpy of Formation
 $\Delta_r H^\circ(\text{Mg}_2\text{TiO}_4, l, 298.15 \text{ K})$ is calculated from $\Delta_r H^\circ(\text{Mg}_2\text{TiO}_4, \text{cr}, 298.15 \text{ K})$ by adding $\Delta_{\text{fus}} H^\circ$ and the difference in enthalpy, $H^\circ(2013 \text{ K}) - H^\circ(298.15 \text{ K})$, between the crystal and liquid.

Heat Capacity and Entropy
 A glass transition is assumed at 1400 K. Below 1400 K the heat capacity is obtained from the heat capacity of the crystal. Above 1400 K the heat capacity is assumed constant and estimated as $54.6 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ or $7.8 \text{ cal} \cdot \text{K}^{-1} \cdot \text{g-atom}^{-1}$. $S^\circ(l, 298.15 \text{ K})$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data
 The incongruent melting point is obtained from Massazza¹ Previous work by Coughanour² suggested congruent melting at 2005 K. $\Delta_{\text{fus}} H^\circ$ is estimated from those of $\text{Na}_2\text{O} \cdot 2\text{TiO}_2$ and $\text{Na}_2\text{O} \cdot \text{TiO}_2$ observed by Naylor³ and $\text{CaO} \cdot \text{TiO}_2$, SiO_2 observed by King.⁴

References
¹F. Massazza and E. Sircchia, 16th Int Congress of Pure and Appl. Chem., Inorg. Sect., Paris (1957), pp 161-8, Butterworths Scientific Publications, London, (1958).
²L. W. Coughanour and V. A. DeProsse, J. Res. Nat. Bur. Stand. 51, 87 (1953).
³B. F. Naylor, J. Amer. Chem. Soc. 67, 2120 (1945).
⁴E. G. King, R. L. Orr and K. R. Bonnickson, J. Amer. Chem. Soc. 76, 4320 (1954).

T/K	C _p ^a	S ^b	[G ^c - H(T)]/T	H ^c - H(T)	Δ _r H ^c	Standard State Pressure = p ^d = 0.1 MPa	log K _f
0							
100							
200							
298.15	128.574	172.412	172.412	0.	-2046.329	-1946.732	341.063
300	129.026	173.209	172.415	0.238	-2046.338	-1946.732	338.832
400	146.285	212.948	177.716	14.093	-2046.150	-1912.729	249.777
500	156.410	246.751	188.230	29.260	-2045.173	-1879.476	196.347
600	163.686	275.939	200.472	45.280	-2043.833	-1846.458	160.748
700	169.582	301.626	213.124	61.952	-2042.303	-1813.681	135.339
800	174.707	324.612	225.648	79.171	-2040.658	-1781.133	116.296
900	179.360	345.462	237.820	96.877	-2038.991	-1748.792	101.497
1000	183.686	364.585	249.553	115.032	-2037.304	-1715.209	89.593
1100	187.778	382.286	260.825	133.607	-2035.214	-1681.336	79.840
1200	191.690	398.793	271.642	152.581	-2033.694	-1647.475	71.713
1300	195.456	414.286	282.025	171.940	-2032.344	-1613.550	64.833
1400	199.091	428.905	291.999	191.668	-2031.581	-1579.481	58.707
1400.000	199.091	428.905	291.999	191.668	GLASS <- -> LIQUID		
1400.000	228.446	428.905	291.999	191.668	TRANSITION		
1500	228.446	444.666	301.658	214.513	-2297.376	-1521.477	52.983
1600	228.446	459.410	311.061	237.357	-2289.228	-1470.019	47.991
1700	228.446	473.259	320.199	260.202	-2281.297	-1419.062	43.602
1800	228.446	486.317	329.069	283.047	-2273.545	-1368.568	39.715
1900	228.446	498.668	337.673	305.891	-2265.985	-1318.498	36.248
2000	228.446	510.386	346.018	328.736	-2257.315	-1268.368	33.126
2013.000	228.446	511.856	347.084	331.706	- - - - CRYSTAL <- -> LIQUID		
2100	228.446	521.532	354.113	351.580	-2266.923	-1218.278	30.303
2200	228.446	532.159	361.966	374.425	-2260.577	-1168.490	27.743
2300	228.446	542.314	369.588	397.270	-2254.277	-1118.992	25.413
2400	228.446	552.037	376.989	420.114	-2248.023	-1069.766	23.283
2500	228.446	561.362	384.179	442.959	-2241.816	-1020.800	21.328
2600	228.446	570.372	391.167	465.804	-2235.654	-972.081	19.529
2700	228.446	578.944	397.963	488.648	-2229.540	-923.598	17.868
2800	228.446	587.252	404.576	511.493	-2223.473	-875.340	16.330
2900	228.446	595.268	411.014	534.338	-2217.453	-827.300	14.901
3000	228.446	603.013	417.286	557.182	-2211.483	-779.465	13.572
3100	228.446	610.504	423.398	580.027	-2205.563	-731.828	12.331
3200	228.446	617.257	429.349	602.872	-2199.695	-684.383	11.171
3300	228.446	624.786	435.175	625.716	-2193.881	-637.130	10.085
3400	228.446	631.696	440.853	648.561	-2188.122	-590.131	9.065
3500	228.446	638.228	446.398	671.405	-2182.422	-543.113	8.106
3600	228.446	644.664	451.817	694.250	-2176.783	-496.355	7.202
3700	228.446	650.923	457.114	717.095	-2171.206	-449.966	6.239
3800	228.446	657.015	462.294	739.939	-2165.693	-403.941	5.282
3900	228.446	662.949	467.364	762.784	-2160.244	-358.261	4.376
4000	228.446	668.733	472.326	785.629	-2154.858	-312.927	3.518

PREVIOUS: June 1961

CURRENT: June 1967

Magnesium Titanium Oxide (Mg₂TiO₄)

Mg₂O₄Ti₂(l)

Magnesium Titanium Oxide (Mg₂TiO₄) CRYSTAL-LIQUID

M_r = 160.4876 Magnesium Titanium Oxide (Mg₂TiO₄)

Mg₂O₄Ti₁(cr,l)

0 to 2013 K crystal
above 2013 K liquid
Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature = T _r = 298.15 K			Standard State Pressure = p° = 0.1 MPa		
	C _p ^o J·K ⁻¹ ·mol ⁻¹	S ^o - (G° - H°(T _r))/T J·K ⁻¹ ·mol ⁻¹	H° - H°(T _r) kJ·mol ⁻¹	Δ _f H° kJ·mol ⁻¹	Δ _f G° kJ·mol ⁻¹	log K _r
0	0	INFINITE	-18.836	-2151.027	-2151.027	INFINITE
100	34.639	26.740	-17.753	-2157.597	-2122.882	1108.880
200	94.520	70.337	-11.113	-2162.710	-2085.881	544.776
298.15	128.574	115.102	0	-2164.383	-2047.719	338.752
300	129.026	115.899	0.238	-2164.393	-2046.995	356.414
400	146.285	155.637	14.093	-2164.204	-2007.859	262.199
500	156.410	189.441	29.260	-2163.228	-1968.873	205.687
600	163.686	218.628	45.280	-2161.887	-1930.126	168.032
700	169.582	244.316	61.952	-2160.357	-1891.618	141.154
800	174.707	267.501	79.171	-2158.713	-1853.339	121.011
900	179.360	288.151	96.877	-2157.045	-1815.267	105.355
1000	183.686	307.275	115.032	-2155.268	-1777.593	92.766
1100	187.778	324.975	133.607	-2153.381	-1740.349	82.452
1200	191.690	341.483	152.581	-2151.398	-1703.567	73.858
1300	195.456	356.976	171.940	-2149.316	-1667.256	66.583
1400	199.091	371.594	191.668	-2147.140	-1631.430	60.118
1500	202.614	385.451	211.754	-2144.872	-1596.107	54.097
1600	206.041	398.637	232.188	-2142.520	-1561.282	48.440
1700	209.367	411.229	252.959	-2140.095	-1526.957	43.112
1800	212.610	423.288	274.058	-2137.608	-1493.138	38.079
1900	215.765	434.868	295.478	-2135.153	-1459.825	33.297
2000	218.840	446.014	317.209	-2132.729	-1426.925	28.818
2013.000	219.233	447.433	320.056	-2132.056	-1426.205	28.448
2013.000	218.446	511.866	449.760	CRYSTAL <- -> LIQUID TRANSITION		
2100	228.446	521.532	469.635	-2266.973	-1218.278	30.303
2200	228.446	532.159	492.480	-2260.577	-1168.490	27.743
2300	228.446	542.314	515.324	-2254.277	-1118.992	25.413
2400	228.446	552.037	538.169	-2248.073	-1069.766	23.283
2500	228.446	561.362	561.013	-2241.816	-1020.800	21.328
2600	228.446	570.372	583.858	-2235.654	-972.081	19.529
2700	228.446	578.944	606.703	-2229.540	-923.588	17.868
2800	228.446	587.257	629.547	-2223.473	-875.340	16.330
2900	228.446	595.268	652.391	-2217.453	-827.300	14.901
3000	228.446	603.013	675.237	-2211.483	-779.465	13.572
3100	228.446	610.504	698.081	-2205.563	-731.828	12.331
3200	228.446	617.757	720.926	-2199.695	-684.383	11.171
3300	228.446	624.786	743.771	-2193.881	-637.120	10.085
3400	228.446	631.606	766.615	-2188.122	-590.031	9.065
3500	228.446	638.228	789.460	-2182.422	-543.113	8.106
3600	228.446	644.664	812.305	-2176.783	-496.355	7.202
3700	228.446	650.923	835.149	-2171.206	-449.656	6.239
3800	228.446	657.015	857.994	-2165.691	-403.011	5.282
3900	228.446	662.949	880.838	-2160.239	-356.424	4.376
4000	228.446	668.733	903.683	-2154.847	-310.000	3.518

PREVIOUS:

CURRENT: June 1967

Magnesium Titanium Oxide (Mg₂TiO₄)

Mg₂O₄Ti₁(cr,l)

CRYSTAL

Magnesium Silicide (Mg₂Si)

$$S^{\circ}(298.15 \text{ K}) = [81.588] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{fus}} = 1375 \text{ K}$$

Enthalpy of Formation

$$\Delta_f H^{\circ}(298.15 \text{ K}) \text{ and } T_{\text{fus}} \text{ from NBS.}^1$$

Heat Capacity and Entropy

$$C_p^{\circ} \text{ and } \Delta_{\text{fus}} H^{\circ} \text{ from Kubaschewski and Evans.}^2 \quad S^{\circ}(298.15 \text{ K}) \text{ estimated.}$$

References

¹U. S. Nat. Bur. Stand., Circ. 500, (1952).

²O. Kubaschewski and E. L. Evans, "Metallurgical Thermochemistry," 3rd ed., Pergamon Press Ltd., New York, (1958).

Magnesium Silicide (Mg₂Si)Mg₂Si₁(cr)

T/K	C _p ^o	S ^o	-(G ^o -H(T))/T	H ^o -H(T)	Δ _f H ^o	Δ _f G ^o	log K _r
0				0.	-77.872	-77.055	13.500
100	67.864	81.588	81.588	0.126	-77.872	-77.055	13.416
200	67.994	82.008	81.589	0.232	-77.872	-77.055	13.416
300	73.764	84.332	84.332	7.232	-77.951	-76.770	10.025
400	77.278	89.683	89.683	14.793	-78.002	-76.468	7.989
500	79.831	95.837	95.837	22.651	-78.054	-76.157	6.630
600	82.006	102.149	102.149	30.745	-78.152	-75.833	5.659
700	83.888	108.335	108.335	39.041	-78.342	-75.491	4.929
800	85.688	114.321	114.321	47.520	-78.661	-75.117	4.360
900	87.404	120.064	120.064	56.175	-96.329	-73.274	3.827
1000	89.077	125.558	125.558	65.000	-97.022	-70.933	3.368
1100	90.667	130.812	130.812	73.987	-97.596	-68.536	2.983
1200	92.257	135.839	135.839	83.134	-98.052	-66.095	2.656
1300	93.850	140.655	140.655	92.439	-98.499	-63.623	2.377
1375.000	93.805	204.996	139.470	90.098	CRYSTAL	LIQUID	---
1400	93.805	206.684	140.655	92.439	-353.209	-57.289	2.137
1500	95.312	213.207	143.277	101.896	-350.734	-56.237	1.262
1600	96.776	219.405	149.718	111.500	-348.152	-55.354	0.501
1700	98.198	225.315	153.992	121.249	-345.645	-54.611	-0.179
1800	99.579	230.967	158.113	131.139	-343.233	-53.999	-0.851
1900	100.918	236.387	162.091	141.164	-340.945	-53.497	-1.449
2000	102.215	241.597	165.937	151.321	-338.765	-53.096	-1.982
2100	103.470	246.615	169.606	161.606	-336.686	-52.786	-2.460
2200	104.684	251.456	173.268	172.014	-334.706	-52.556	-2.891
2300	105.855	256.136	176.770	182.541	-332.826	-52.396	-3.281
2400	106.985	260.665	180.172	193.183	-331.046	-52.296	-3.634
2500	108.073	265.054	183.480	203.936	-329.366	-52.246	-3.956

PREVIOUS

CURRENT: December 1960

Magnesium Silicide (Mg₂Si)Mg₂Si₁(cr)

Magnesium Silicide (Mg₂Si)

S°(298.15 K) = [123.472] J·K⁻¹·mol⁻¹
 T_{fus} = 1375 K

Enthalpy of Formation

Δ_fH°(Mg₂Si, l, 298.15 K) is calculated from Δ_fH°(Mg₂Si, cr, 298.15 K) by adding Δ_{sub}H° and the difference in enthalpy, F°(1375 K) - H°(298.15 K), between the crystal and liquid.

Fusion Data

T_{fus} from: ¹Δ_{sub}H° from Kubaschewski and Evans.² Other data estimated.

References

- ¹U. S. Nat. Bur. Stand., Circ. 500, (1952).
- ²O. Kubaschewski and E. L. Evans, "Metallurgical Thermochemistry", 3rd ed., Pergamon Press. Ltd., New York, (1958).

LIQUID

M_r = 76.6955 Magnesium Silicide (Mg₂Si)

$$\Delta_f H^\circ(298.15 \text{ K}) = [-3.372] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_{\text{sub}} H^\circ = [85.772] \text{ kJ}\cdot\text{mol}^{-1}$$

T/K	C _p ^o	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = P° = 0.1 MPa			
		S° - [G° - F°(T _r)]/T	H° - H°(T _r)	Δ _f H°	Δ _f G°		
		J·K ⁻¹ ·mol ⁻¹	J·mol ⁻¹	kJ·mol ⁻¹	log K _r		
0							
100							
200							
298.15	94.140	123.472	123.472	0.	-3.377	-15.048	2.636
300	94.140	124.054	123.474	0.174	-3.282	-15.121	2.633
400	94.140	151.126	171.166	9.588	-1.100	-19.408	2.534
500	94.140	172.143	134.139	19.002	0.703	-24.201	2.528
600	94.140	189.307	141.947	28.416	2.206	-29.327	2.553
700	94.140	203.819	149.776	37.830	3.428	-34.683	2.588
800	94.140	216.389	157.334	47.244	4.357	-40.195	2.624
900	94.140	227.477	164.524	56.658	4.971	-45.844	2.658
1000	94.140	237.396	171.324	66.072	-11.938	-50.039	2.614
1100	94.140	246.369	177.745	75.486	-12.041	-53.844	2.557
1200	94.140	254.560	183.810	84.900	-12.188	-57.638	2.509
1300	94.140	262.095	189.546	94.314	-12.376	-61.418	2.468
1375.000	94.140	267.375	193.648	101.375	---	CRYSTAL ← --> LIQUID	---
1400	94.140	269.072	194.980	103.728	-267.425	-58.848	2.196
1500	94.140	275.567	200.138	113.142	-264.992	-44.035	1.533
1600	94.140	281.642	205.045	122.556	-262.602	-29.383	0.959
1700	94.140	287.349	209.720	131.970	-310.430	-14.432	0.443
1800	94.140	292.730	214.184	141.384	-307.893	2.906	-0.084
1900	94.140	297.820	218.453	150.798	-305.356	20.104	-0.553
2000	94.140	302.649	222.543	160.212	-302.819	37.168	-0.971
2100	94.140	307.242	226.468	169.626	-300.282	54.105	-1.346
2200	94.140	311.621	230.040	179.040	-297.747	70.921	-1.684
2300	94.140	315.806	233.870	188.454	-295.212	87.622	-1.990
2400	94.140	319.813	237.568	197.868	-292.679	104.212	-2.268
2500	94.140	323.636	240.743	207.282	-290.148	120.697	-2.522
2600	94.140	327.348	244.003	216.696	-287.621	137.081	-2.754
2700	94.140	330.901	247.156	226.110	-285.098	153.368	-2.967
2800	94.140	334.324	250.209	235.524	-282.582	169.562	-3.163
2900	94.140	337.628	253.167	244.938	-280.074	185.665	-3.344
3000	94.140	340.819	256.035	254.352	-277.576	201.683	-3.512
3100	94.140	343.906	258.820	263.766	-275.091	217.617	-3.667
3200	94.140	346.895	261.526	273.180	-272.623	233.471	-3.811
3300	94.140	349.792	264.157	282.594	-270.173	249.249	-3.945
3400	94.140	352.602	266.718	292.008	-267.745	264.952	-4.070
3500	94.140	355.331	269.211	301.422	-265.344	280.585	-4.188
3600	94.140	357.983	271.640	310.836	-262.961	296.114	-4.299
3700	94.140	360.563	274.008	320.250	-260.596	311.563	-4.402
3800	94.140	363.073	276.319	329.664	-258.252	326.943	-4.491
3900	94.140	365.518	278.575	339.078	-255.928	342.256	-4.571
4000	94.140	367.902	280.779	348.492	-253.626	357.519	-4.643

PREVIOUS:

CURRENT: December 1960

Magnesium Silicide (Mg₂Si)

Mg₂Si(l)

Magnesium Silicide (Mg₂Si) CRYSTAL-LIQUID

M_r = 76.6955 Magnesium Silicide (Mg₂Si)

Mg₂Si_l(cr.l)

0 to 1375 K crystal
above 1375 K liquid

Refer to the individual tables for details.

T/K	C _p ^a	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p ^o = 0.1 MPa		log K _r
		S ^o - [G ^o - H ^o (T _r)]/T	H ^o - H ^o (T _r)	ΔH ^o	ΔG ^o	
		J · K ⁻¹ · mol ⁻¹		kJ · mol ⁻¹		
0						
100						
200						
298.15	67.864	81.588	81.588	0.	-77.822	-77.055
300	67.994	82.008	81.589	0.126	-77.826	-77.050
400	73.764	102.413	84.332	7.232	-77.951	-76.770
500	77.278	119.268	89.683	14.793	-78.002	-76.468
600	79.831	133.589	95.837	22.651	-78.054	-76.157
700	82.006	146.062	102.140	30.745	-78.152	-75.833
800	83.889	157.137	108.335	39.041	-78.342	-75.491
900	85.688	167.122	114.321	47.520	-78.661	-75.117
1000	87.404	176.239	120.064	56.175	-79.274	-73.827
1100	89.077	184.649	125.558	65.000	-80.022	-70.933
1200	90.567	192.468	130.812	73.987	-80.956	-68.536
1300	92.257	199.788	135.839	83.134	-82.052	-66.095
1375.000	93.450	204.996	139.470	90.098	-83.370	-63.500
1400	94.140	207.375	139.470	175.870	-83.370	-63.500
1500	94.140	269.072	141.769	178.223	-267.425	-38.848
1600	94.140	275.567	150.475	187.637	-264.992	-44.035
1700	94.140	281.642	158.485	197.051	-262.602	-49.383
1800	94.140	287.349	165.899	206.465	-260.260	-54.883
1900	94.140	292.730	172.797	215.879	-257.967	-60.533
2000	94.140	297.820	179.245	225.293	-255.723	-66.343
2100	94.140	302.649	185.295	234.707	-253.529	-72.313
2200	94.140	307.242	190.984	244.121	-251.375	-78.443
2300	94.140	311.621	196.378	253.535	-249.261	-84.723
2400	94.140	315.806	201.489	262.849	-247.187	-91.153
2500	94.140	319.813	206.328	272.163	-245.163	-97.733
2600	94.140	323.656	210.945	281.577	-243.189	-104.463
2700	94.140	327.348	215.351	291.191	-241.265	-111.343
2800	94.140	330.901	219.566	300.605	-239.391	-118.373
2900	94.140	334.324	223.603	310.019	-237.567	-125.553
3000	94.140	337.628	227.479	319.433	-235.793	-132.883
3100	94.140	340.819	231.204	328.847	-234.069	-140.363
3200	94.140	343.906	234.790	338.261	-232.395	-147.893
3300	94.140	346.895	238.247	347.675	-230.771	-155.473
3400	94.140	349.792	241.583	357.089	-229.197	-163.103
3500	94.140	352.602	244.807	366.503	-227.673	-170.783
3600	94.140	355.331	247.976	375.917	-226.199	-178.513
3700	94.140	357.983	250.947	385.331	-224.775	-186.293
3800	94.140	360.563	253.875	394.745	-223.401	-194.123
3900	94.140	363.073	256.715	404.159	-222.077	-202.003
4000	94.140	365.518	259.474	413.573	-220.803	-210.033
		367.902	262.155	422.987	-219.579	-218.213

PREVIOUS:

CURRENT: December 1960

Magnesium Silicide (Mg₂Si)

Mg₂Si_l(cr.l)

Mg₃N₂(cr)

Mg₃N₂(cr)

CRYSTAL

Magnesium Nitride (Mg₃N₂)

$S^\circ(298.15\text{ K}) = [87.864 \pm 8.4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

$\Delta_f H^\circ(298.15\text{ K}) = -461.08 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$ Standard State Pressure = $p^\circ = 0.1\text{ MPa}$

Enthalpy of Formation
Data from Douglas *et al.*¹

Heat Capacity and Entropy
Data from Douglas *et al.*¹

Reference

¹F. B. Douglas, A. C. Victor, and A. R. Beaudoin, U. S. Nat. Bur. Stand., Report 6928, Appendix B, (1960).

T/K	C _p ^o	S ^o	-[G ^o -H ^o (T _r)]/T	H ^o -H ^o (T _r)	Δ _f H ^o	Δ _f G ^o	log K _r
0							
100							
200							
298.15	104.516	87.864	87.864	0.	-461.077	-400.923	70.240
300	104.600	88.511	87.866	0.193	-461.075	-400.549	69.742
400	107.654	119.021	92.005	10.806	-461.046	-380.381	49.673
500	110.709	143.371	95.922	21.724	-461.067	-360.213	37.653
600	113.763	163.826	108.913	32.948	-461.128	-340.037	29.603
700	116.817	181.592	118.053	44.477	-461.258	-319.846	23.667
800	119.872	197.390	127.001	56.311	-461.498	-299.630	19.564
823.000	120.574	200.797	129.016	59.076			
823.000	123.846	201.916	129.016	59.997			
900	123.846	212.993	135.733	69.533	-460.808	-279.470	16.220
1000	123.846	226.041	144.123	81.918	-487.232	-257.154	13.432
1061.000	123.846	233.374	149.046	89.472			
1061.000	123.595	234.399	149.046	90.560			
1100	123.595	238.861	152.152	95.380	-487.359	-234.128	11.118
1200	123.595	249.615	159.832	107.740	-488.441	-211.020	9.187
1300	123.595	259.508	167.124	120.100	-489.968	-187.864	7.348
1400	123.595	268.668	174.054	132.149	-493.563	-155.072	5.786
1500	123.595	277.193	180.649	144.819	-497.908	-103.843	3.616
1600	123.595	285.171	186.935	157.178	-868.283	-52.793	1.724
1700	123.595	292.664	192.936	169.538	-865.684	-1.905	0.059
1800	123.595	299.729	198.675	181.897	-863.110	48.831	-1.417
1900	123.595	306.411	204.171	194.257	-860.556	99.425	-2.733
2000	123.595	312.751	209.443	206.616	-858.022	149.885	-3.915
2100	123.595	318.781	214.507	218.976	-855.504	200.218	-4.980
2200	123.595	324.531	219.378	231.335	-853.002	250.432	-5.946
2300	123.595	330.025	224.071	243.695	-850.516	300.532	-6.825
2400	123.595	335.285	228.596	256.054	-848.043	350.524	-7.679
2500	123.595	340.330	232.965	268.414	-845.586	400.414	-8.566

PREVIOUS:

CURRENT: December 1960

Magnesium Nitride (Mg₃N₂)

Mg₃N₂(cr)

Magnesium Phosphate ($Mg_3P_2O_8$)

CRYSTAL

 $M_r = 262.85772$

$S^\circ(298.15\text{ K}) = [188.280] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $T_{\text{fus}} = 1621 \text{ K}$
 $\Delta_f H^\circ(298.15\text{ K}) = -3745.10 \pm 10.5 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{ion}} H^\circ = [121.336 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_f H^\circ(0\text{ K}) = \text{Unknown}$

Enthalpy of Formation

The selected $\Delta_f H^\circ(298.15\text{ K})$ is a weighted average of a revised calorimetric determination and a 3rd law calculation using equilibrium data. A calorimetric determination of the enthalpy of formation reported by Stevens and Turkdogan¹ was revised three ways:

1. The enthalpy of reaction for the reaction $3\text{MgO}(\text{cr}) + \text{P}_2\text{O}_5(\text{orthorhombic}) \rightarrow \text{Mg}_3\text{P}_2\text{O}_8(\text{cr})$ had been evaluated at 348 K. A small temperature correction to 298.15 K was made with thermal data not available to Stevens and Turkdogan¹ on MgO (Giauque (2)), P_2O_5 JANAF Table, December 31, 1962) and $\text{Mg}_3\text{P}_2\text{O}_8$ (this table).

2. A new $\Delta_f H^\circ(298.15\text{ K})$ for $\text{P}_2\text{O}_5(\text{hexagonal})$ as reported by Holmes³ was combined with the enthalpy of reaction, $-6.85 \pm 1.0 \text{ kcal}\cdot\text{mol}^{-1}$, for the reaction $\text{P}_2\text{O}_5(\text{hexagonal}) \rightarrow \text{P}_2\text{O}_5(\text{orthorhombic})$ as reported by Hill *et al.*⁴.

3. A correction of $+8.35 \text{ kcal}\cdot\text{mol}^{-1}$ was made for the change in phosphorus reference state from white (α) to red (β). (The correction is $+8.35 \text{ kcal}\cdot\text{mol}^{-1}$ of $\text{Mg}_3\text{P}_2\text{O}_8$ or $+4.173 \text{ kcal}\cdot\text{mol}^{-1}$ of P_2O_5 .)

This revised $\Delta_f H^\circ(298.15\text{ K})$, $897.60 \pm 2.0 \text{ kcal}\cdot\text{mol}^{-1}$, would appear to be more reliable than the original value reported by Stevens and Turkdogan¹.

For the reaction $\text{Mg}_3\text{P}_2\text{O}_8(\text{cr}) + 5 \text{H}_2(\text{g}) \rightarrow 3 \text{MgO}(\text{cr}) + \text{P}_2(\text{g}) + 5 \text{H}_2\text{O}(\text{g})$, the 3rd law treatment of the equilibrium data of Bookley⁵ and the JANAF table free energy functions gave a $\Delta_f H^\circ(298.15\text{ K}) = -893.11 \text{ kcal}\cdot\text{mol}^{-1}$.

The quantity, $-895.10 \pm 2.50 \text{ kcal}\cdot\text{mol}^{-1}$, is taken as the most probable value for the enthalpy of formation of magnesium orthophosphate.

Heat Capacity and Entropy

The entropy at 298.15 K was estimated by considering the additive entropy constants of Kelley⁶ and Evans and Kubaschewski.⁷ The heat capacity was estimated in a similar manner by considering the heat capacities of the constituent elements and related compounds such as MgO , Mg , P_2O_5 , $\text{Ca}_3\text{P}_2\text{O}_7$, and $\text{Ca}_3\text{P}_2\text{O}_8$.

Fusion Data

The melting point, 1621 K, as reported by Stevens and Turkdogan¹ was selected. There is disagreement on the melting point in the literature. From the work of Winter,⁸ Kelley⁹ has quoted a melting point of 1457 K and has calculated a "rather uncertain value" of 11,300 $\text{kcal}\cdot\text{mol}^{-1}$ for the heat of fusion. Bookley⁵ has found a melting point of 1703 K. Berak¹⁰ gives 1630 K as the melting point.

References

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- K. K. Kelley, U. S. Bur. Mines, personal communication, (June 1960).
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Magnesium Phosphate ($Mg_3P_2O_8$) $Mg_3O_8P_2(\text{cr})$

T/K	C _v ^a	S ^b	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p ^c = 0.1 MPa		log K _r
			$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_r G^\circ$	
0							
100							
200							
298.15	212.756	188.280	188.280	0.	-3745.098	-3502.859	613.686
300	213.384	189.598	188.284	0.394	-3745.148	-3501.356	609.640
400	240.162	254.762	196.988	23.110	-3748.487	-3419.389	446.528
500	262.337	310.777	214.270	48.254	-3748.843	-3337.054	348.620
600	282.211	360.377	234.563	75.488	-3747.814	-3254.772	283.353
700	301.248	405.305	255.793	104.638	-3745.544	-3172.761	236.754
800	320.620	446.840	277.109	135.783	-3741.994	-3091.163	201.832
900	335.975	485.488	298.140	168.613	-3737.409	-3010.075	174.700
1000	351.540	521.734	318.706	203.048	-3731.656	-2927.411	152.912
1100	360.075	555.683	338.726	238.653	-3751.645	-2844.671	135.082
1200	365.682	587.236	358.136	274.970	-3872.275	-2760.346	120.155
1300	373.757	616.851	376.909	311.975	-3863.611	-2668.032	107.203
1400	377.899	644.714	395.053	349.575	-4236.710	-2566.904	95.772
1500	379.907	670.862	412.578	387.425	-4223.344	-2448.098	85.250
1600	380.744	695.407	429.496	425.458	-4209.957	-2330.185	76.073
1621.000	380.920	700.373	432.973	433.453	---	---	---
1700	381.581	718.517	445.824	463.578	-4196.587	-2213.109	68.001
1800	381.581	740.328	461.585	501.736	-4183.281	-2096.819	60.848
1900	381.581	760.959	476.804	539.894	-4170.074	-1981.265	54.469
2000	381.581	780.531	491.505	578.052	-4156.965	-1866.404	48.745
2100	381.581	799.149	508.715	616.210	-4143.953	-1752.196	43.583
2200	381.581	816.900	519.460	654.368	-4131.056	-1638.604	38.905
2300	381.581	833.862	532.763	692.526	-4118.215	-1525.600	34.647
2400	381.581	850.107	545.650	730.683	-4105.489	-1413.152	30.756
2500	381.581	865.679	558.142	768.843	-4092.858	-1301.251	27.188
2600	381.581	880.644	570.260	807.001	-4080.321	-1189.814	23.904
2700	381.581	895.045	582.024	845.159	-4067.878	-1078.876	20.872
2800	381.581	908.923	593.452	883.317	-4055.529	-968.398	18.066
2900	381.581	922.313	604.563	921.475	-4043.276	-858.362	15.461
3000	381.581	935.249	615.371	959.633	-4031.118	-748.744	13.037

PREVIOUS: December 1960

CURRENT: March 1963

Magnesium Phosphate ($Mg_3P_2O_8$) $Mg_3O_8P_2(\text{cr})$

Magnesium Phosphate (Mg₃P₂O₈)

LIQUID

Magnesium Phosphate (Mg₃P₂O₈)

Mg₃O₈P₂(l)

S°(298.15 K) = [235.102] J·K⁻¹·mol⁻¹
T_{liq} = 1621 K

Δ_fH°(298.15 K) = [-3663.190] kJ·mol⁻¹
Δ_{liq}H° = [121.336 ± 41.8] kJ·mol⁻¹

Enthalpy Reference Temperature = T_r = 298.15 K

Standard State Pressure = p° = 0.1 MPa

Enthalpy of Formation

Δ_fH°(Mg₃P₂O₈, l, 298.15 K) is calculated from Δ_fH°(Mg₃P₂O₈, cr, 298.15 K) by adding Δ_{liq}H° and the difference in enthalpy, H°(1621 K) - H°(298.15 K), between the crystal and liquid.

Heat Capacity and Entropy

The heat capacity was estimated as 13/11 of the corresponding heat capacity of Ca₃P₂O₇ as given in Kelley,¹ S°(l, 298.15 K) is calculated in a manner similar to that used for the enthalpy of formation.

Fusion Data

The enthalpy of fusion was estimated by taking 13/11 of the Δ_{liq}H° of Ca₃P₂O₇ as given in Kelley.¹

Reference

¹K. K. Kelley, U. S. Bur. Mines Bull. 5841, (1960).

T/K	C _p ^o	S ^o	-(G° - H°(T _r))/T	H° - H°(T _r)	Δ _f H°	log K _f
0				0.		
100	212.756	235.102	235.102	0.	-3663.190	601.782
200	213.384	236.420	235.106	0.394	-3663.240	597.824
300	240.162	357.584	243.810	23.110	-3666.578	438.277
400	262.337	407.199	261.092	48.254	-3666.934	342.508
500	282.211	452.127	281.385	75.488	-3665.905	278.658
600	301.748	493.663	302.615	104.658	-3663.635	233.088
700	320.670	532.311	324.931	135.785	-3660.086	198.930
800	335.975	568.576	344.963	168.613	-3655.500	171.392
900	351.540	602.505	365.529	203.048	-3675.747	151.080
1000	360.075	634.097	385.548	238.653	-3669.736	133.638
1200	365.682	640.148	408.766	274.965	-3790.321	119.035
1220.000	366.451	640.148	408.766	282.287	GLASS <- -> LIQUID	
1220.000	366.451	640.148	408.766	282.287	TRANSITION	
1300	475.302	670.336	423.944	320.311	-3773.316	106.369
1400	475.302	705.560	441.817	367.841	-4136.486	95.711
1500	475.302	738.353	461.439	415.371	-4115.490	84.950
1600	475.302	769.028	479.715	462.901	-4090.605	76.022
1621.000	475.302	775.226	483.503	472.883	CRYSTAL <- -> LIQUID	
1700	475.302	797.843	497.589	510.432	-4067.825	68.188
1800	475.302	825.011	515.032	557.962	-4045.146	61.263
1900	475.302	850.769	532.329	603.492	-4022.588	54.102
2000	475.302	875.089	548.577	653.022	-4000.086	49.587
2100	475.302	898.279	564.682	700.553	-3977.702	44.626
2200	475.302	920.390	580.352	748.083	-3955.413	40.141
2300	475.302	941.518	595.599	795.613	-3933.220	36.069
2400	475.302	961.747	610.437	843.143	-3911.122	32.358
2500	475.302	981.149	624.880	890.674	-3889.119	28.962
2600	475.302	999.791	638.943	938.204	-3867.209	25.846
2700	475.302	1017.729	652.642	985.734	-3845.394	22.976
2800	475.302	1035.015	665.992	1033.264	-3823.673	20.327
2900	475.302	1051.694	679.006	1080.795	-3802.047	17.874
3000	475.302	1067.807	691.699	1128.325	-3780.518	15.598
3100	475.302	1083.392	704.084	1175.855	-3759.085	13.480
3200	475.302	1098.482	716.175	1223.383	-3737.751	11.506
3300	475.302	1113.108	727.982	1270.916	-3716.518	9.643
3400	475.302	1127.298	739.519	1318.446	-3695.387	7.937
3500	475.302	1141.075	750.797	1365.976	-3674.363	6.320
3600	475.302	1154.465	761.824	1413.506	-3653.448	4.801
3700	475.302	1167.488	772.613	1461.036	-3632.647	3.372
3800	475.302	1180.163	783.172	1508.567	-3611.963	2.026
3900	475.302	1192.510	793.510	1556.097	-3591.401	0.757
4000	475.302	1204.543	803.636	1603.627	-3570.967	-0.442
4100	475.302	1216.280	813.558	1651.157	-3550.666	-1.576
4200	475.302	1227.733	823.284	1698.688	-3530.503	-2.650
4300	475.302	1238.918	832.820	1746.218	-3510.485	-3.669
4400	475.302	1249.844	842.174	1793.748	-3490.617	-4.635
4500	475.302	1260.526	851.353	1841.278	-3470.904	-5.553

PREVIOUS: December 1960

CURRENT: March 1963

Magnesium Phosphate (Mg₃P₂O₈)

Mg₃O₈P₂(l)

0 to 1621 K crystal
above 1621 K liquid
Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa		$\log K_r$
	C_p°	$S^\circ - [C_p^\circ - H^\circ(T)]/T$	$H^\circ - H^\circ(T)$	$\Delta_f H^\circ$	
0			0		
100			0.394	-3745.098	613.686
200			23.110	-3748.487	609.640
298.15	212.756	188.280	48.254	-3748.843	466.528
300	213.384	189.598	75.488	-3747.814	348.620
400	240.162	196.988	104.658	-3745.544	283.353
500	262.337	214.270	135.785	-3741.994	236.754
600	282.211	234.563	168.613	-3737.409	201.832
700	301.248	255.793	203.048	-3737.656	174.700
800	320.620	277.109	238.653	-3751.645	152.912
900	335.975	298.140	274.920	-3872.275	135.082
1000	351.540	318.706	311.925	-4236.710	120.155
1100	360.075	338.726	359.525	-4723.344	107.203
1200	365.682	358.136	387.425	-4209.957	95.772
1300	373.757	376.909	435.455	-2330.185	85.250
1400	377.899	644.714	433.455		76.073
1500	379.907	412.578	432.973		
1600	380.744	695.407	432.973		
1621.000	380.920	700.373	432.973		
1621.000	475.302	775.226	432.973		
1700	475.302	797.843	592.340	-4067.825	68.188
1800	475.302	825.011	639.870	-4045.147	61.263
1900	475.302	850.709	687.401	-4022.568	55.102
2000	475.302	875.089	734.931	-4000.086	49.587
2100	475.302	898.279	782.461	-3977.702	44.626
2200	475.302	920.390	829.991	-3955.413	40.141
2300	475.302	941.518	877.522	-3933.220	36.069
2400	475.302	961.747	925.052	-3911.122	32.338
2500	475.302	981.149	972.582	-3889.119	28.962
2600	475.302	999.791	1020.112	-3867.209	25.846
2700	475.302	1017.729	1067.643	-3845.394	22.976
2800	475.302	1035.015	1115.173	-3823.673	20.327
2900	475.302	1051.694	1162.703	-3802.047	17.874
3000	475.302	1067.807	1210.233	-3780.518	15.598
3100	475.302	1083.392	1257.764	-3759.085	13.480
3200	475.302	1098.482	1305.294	-3737.751	11.506
3300	475.302	1113.108	1352.824	-3716.518	9.663
3400	475.302	1127.298	1400.354	-3695.387	7.937
3500	475.302	1141.075	1447.885	-3674.363	6.320
3600	475.302	1154.465	1495.415	-3653.448	4.801
3700	475.302	1167.488	1542.945	-3632.647	3.372
3800	475.302	1180.163	1590.476	-3611.963	2.022
3900	475.302	1192.510	1638.006	-3591.401	0.757
4000	475.302	1204.543	1685.536	-3570.967	-0.442
4100	475.302	1216.280	1733.066	-3550.666	-1.576
4200	475.302	1227.733	1780.596	-3530.503	-2.650
4300	475.302	1238.917	1828.126	-3510.485	-3.669
4400	475.302	1249.844	1875.657	-3490.617	-4.635
4500	475.302	1260.526	1923.187	-3470.904	-5.553

PREVIOUS:

CURRENT: March 1963

Magnesium

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