

## Beryllium (Be)

## REFERENCE STATE

 $A_t = 9.01218$  Beryllium (Be)Be<sub>t</sub>(ref)

0	to	1527	K crystal, alpha
1527	to	1560	K crystal, beta
1560	to	2741.437	K liquid
above		2741.437	K ideal monatomic gas

Refer to the individual tables for details.

T/K	C <sub>p</sub> JK <sup>-1</sup> mol <sup>-1</sup>	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $P^* = 0.1$ MPa	
		S <sup>*</sup> J K <sup>-1</sup> mol <sup>-1</sup>	-[G <sup>*</sup> -H <sup>r</sup> (T)]/T	H <sup>r</sup> -H <sup>r</sup> (T)/T kJ mol <sup>-1</sup>	$\Delta H^*$ kJ mol <sup>-1</sup>
0	0	0	0	-1.932	0
100	1.819	0.503	19.454	-1.893	0
200	9.984	4.174	10.751	-1.315	0
298.15	16.380	9.440	9.440	0	0
300	16.472	9.542	9.440	0.030	0
400	19.965	14.817	10.136	1.872	0
500	21.943	19.501	11.551	3.975	0
600	23.336	23.630	13.227	6.242	0
700	24.463	27.314	14.981	8.634	0
800	25.458	30.647	16.734	11.130	0
900	26.384	33.699	18.452	13.723	0
1000	27.274	36.525	20.119	16.406	0
1100	28.147	39.166	21.732	19.177	0
1200	29.016	41.632	23.290	21.035	0
1300	29.886	44.009	24.793	24.980	0
1400	30.763	46.256	26.247	28.013	0
1500	31.630	48.409	27.653	31.133	0
1527.000	31.892	48.975	28.025	31.991	—
1527.000	30.000	53.461	28.025	38.840	—
1560.000	30.000	54.102	28.570	39.830	—
1560.000	28.788	59.163	28.570	47.725	—
1600	28.874	59.893	29.344	48.879	0
1700	29.089	61.650	31.193	51.777	0
1800	29.304	63.319	32.932	54.696	0
1900	29.519	64.999	34.573	57.638	0
2000	29.734	66.429	36.128	60.600	0
2100	29.949	67.884	37.606	63.584	0
2200	30.164	69.283	39.014	66.590	0
2300	30.379	70.628	40.360	69.617	0
2400	30.594	71.926	41.648	72.666	0
2500	30.809	73.179	42.885	75.736	0
2600	31.024	74.391	44.073	78.828	0
2700	31.239	75.566	45.218	81.941	0
2741.437	31.328	76.043	45.680	83.257	—
2741.437	20.883	182.400	45.680	374.809	—
2800	20.905	182.842	48.545	376.032	—
2900	20.949	183.576	53.188	378.125	—
3000	21.006	184.287	57.546	380.223	—
3100	21.076	184.977	61.646	382.327	—
3200	21.159	185.648	65.511	384.438	—
3300	21.259	186.300	69.161	386.559	—
3400	21.376	186.937	72.616	388.691	—
3500	21.512	187.538	75.391	390.835	—
3600	21.668	188.166	79.001	392.994	—
3700	21.844	188.762	81.960	393.169	—
3800	22.041	189.347	84.778	397.263	—
3900	22.239	189.923	87.487	399.578	—
4000	22.500	190.489	90.035	401.816	—
4100	22.761	191.048	92.492	404.079	—
4200	23.045	191.600	94.845	406.360	—
4300	23.349	192.146	97.102	408.588	—
4400	23.674	192.686	99.268	411.039	—
4500	24.019	193.222	101.350	413.424	—
4600	24.383	193.754	103.345	415.844	—
4700	24.764	194.292	105.252	418.201	—
4800	25.162	194.808	107.142	420.797	—
4900	25.576	195.331	108.926	423.334	—
5000	26.003	195.852	110.669	425.913	—
5200	26.894	196.889	113.945	431.202	—
5400	27.822	197.921	117.036	436.673	—
5600	28.776	198.950	119.962	442.332	—
5800	29.743	199.977	122.704	448.184	—
6000	30.711	201.001	125.297	454.229	—

CURRENT: September 1983 (1 bar)

PREVIOUS: September 1961 (1 atm)  
Beryllium (Be) Be<sub>t</sub>(ref)

CRYSTAL( $\alpha$ - $\beta$ ) $A_r = 9.01218$  Beryllium (Be)

## Beryllium (Be)

 $\text{Be}_1(\text{cr})$ 

$$\begin{aligned} S^\circ(298.15 \text{ K}) &= 9.44 \pm 0.15 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1} \\ \Delta_n H^\circ &= 4527 \pm 25 \text{ K} \quad (\alpha \rightarrow \beta) \\ T_{\text{fus}} &= 1560 \pm 5 \text{ K} \quad (\beta \rightarrow \text{l}) \end{aligned}$$

**Enthalpy of Formation**  
Zero by definition.

**Heat Capacity and Entropy**

The adopted thermal functions for Be( $\alpha$ ,  $\beta$ , cr) are derived from the studies of Ahlers (1.4–30 K),<sup>1</sup> Hill and Smith (4–300 K),<sup>2</sup> Ginnings<sup>3</sup> et al. (367–1169 K),<sup>3</sup> and Kantor et al. (600–3200 K).<sup>4</sup> The mathematical and graphical treatment of these four studies yields a continuous and smooth heat capacity curve for  $\alpha$ -Be(cr).

There are no heat capacity or enthalpy measurements for  $\beta$ -Be(cr). We assume a constant value of  $C_p = 30.0 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  for the  $\beta$ -region.

The entropy at 29.15 K is  $0.06 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  less than that recommended by CODATA.<sup>5</sup> This is undoubtedly due to the manner in which the data of Ahlers<sup>1</sup> and Hill and Smith<sup>2</sup> were merged. A detailed discussion of the heat capacities of all alkaline earth metals is in preparation.

**Phase and Fusion Data**

Canion<sup>6</sup> has summarized the data on the polymorphic phase changes and the variation of the melting temperature of beryllium with pressure. His critical evaluation results in the recommendation that at ambient pressure there are two stable phases. His recommendations are entirely attributable to the resistance studies of Francois and Conire.<sup>7</sup> The phases are denoted alpha(ahcp) and beta(bcc).

The melting point of beryllium is fairly well defined. We adopt  $T_{\text{fus}} = 1560 \pm 5 \text{ K}$  based on the studies of Kantor et al.,<sup>4</sup> Martin and Moore,<sup>8</sup> Teitel and Cohen,<sup>9</sup> and Loasby and Dearden.<sup>10</sup>

The alpha-beta transition is ill-defined. There are many conflicting studies as to the value of the transition temperature and the value and sign of the derivative  $(dT/dP)$  for this transition. We adopt  $T_{\text{ts}} = 1527 \pm 25 \text{ K}$  based on the study of Ammonenko, et al.<sup>11</sup>

The enthalpies of transition and fusion are also poorly defined. Kantor, et al.<sup>4</sup> has measured the enthalpy of the crystal and liquid. No data points were obtained in the beta phase region. As a result, we can only derive a combined value for the enthalpy of transition and fusion. Following the suggestion of Abey,<sup>12</sup> the enthalpy values of Loasby and Dearden<sup>10</sup> and Abey<sup>13</sup> have the same value for the ratio of the transition enthalpy to fusion enthalpy, even though the actual values for each enthalpy are quite different. Thus, using this ratio and the sum of the enthalpies, as determined by Kantor et al.,<sup>4</sup> we calculate the individual enthalpies of transition and fusion. A much more detailed discussion is in progress.

**Sublimation Data**

Refer to the ideal gas table for details.

**References**

- <sup>1</sup>G. Ahlers, Phys. Rev. **145**, 419 (1966).
- <sup>2</sup>R. W. Hill and P. L. Smith, Phil. Mag. **44**, 636 (1953).
- <sup>3</sup>D. C. Ginnings, T. B. Douglas, and A. F. Ball, J. Am. Chem. Soc. **73**, 1236 (1951).
- <sup>4</sup>P. B. Kantor, R. M. Krasovskaya, and A. N. Kisel, Fiz. Metal. i. Metalloved., Akad. Nauk SSSR **10**, 835 (1960) [Phys. Metals Metallogr. **10** (6), 42 (1960)].
- <sup>5</sup>J. D. Cox, Chairman, ICSU-CODATA Task Group on Key Values for Thermodynamics, J. Chem. Thermodyn. **10**, 903 (1978).
- <sup>6</sup>J. F. Canion, J. Phys. Chem. Ref. Data **3**, 781 (1974).
- <sup>7</sup>M. Francois and M. Conire, Conf. Int. Met. Beryllium, Commun., 3rd, pp. 201–11, (1965).
- <sup>8</sup>A. J. Martin and A. Moore, J. Less-Common Metals **1**, 85 (1959).
- <sup>9</sup>R. J. Teitel and M. Cohen, J. Met. **185**, 285 (1949).
- <sup>10</sup>R. G. Loasby and D. Dearden, J. Less-Common Metals **52**, 137 (1977).
- <sup>11</sup>V. M. Amonenko, V. E. Ivanov, et al., Phys. Metals Metallogr. **12**, 77 (1962).
- <sup>12</sup>A. Abey, Lawrence Livermore National Laboratory, UCRL-533567, (1984).

PREVIOUS September 1961

CURRENT: September 1983

## Beryllium (Be)

## Be(I)

A<sub>r</sub> = 9.01218 Beryllium (Be)

## LIQUID Beryllium (Be)

$$S^o(298.15\text{ K}) = [19.539] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{us} = 1560 \pm 5 \text{ K } (\beta \rightarrow)$$

**Enthalpy of Formation**  
The enthalpy of formation of liquid beryllium is calculated from that of the crystal by adding  $\Delta_{us}H^o$  and the difference in enthalpy,  $H^o(1560 \text{ K}) - H^o(298.15 \text{ K})$ , between the crystal and liquid.

**Heat Capacity and Entropy**

The heat capacity of the liquid is derived from the measured enthalpy data of Kantor *et al.*,<sup>1</sup> 17 data points in the liquid region, 1560 to 2200 K. The data was presented graphically. We adopt the reported equation:  $C_p^o = 6.079 + 5.138 \times 10^{-4} T \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . This equation is used to calculate extrapolated values from 2200 K to 3500 K and from 1150 K to 1560 K.

A glass transition temperature is assumed at 1150 K, below which the heat capacity values of crystalline beryllium are adopted. The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

**Transition and Fusion Data**  
Refer to the crystal table for details.**Vaporization Data**

There is only one reported vaporization study for Be(0): Baur and Brunner (926–1283 K).<sup>2</sup> This study was not considered in the analysis as it had an incorrect temperature dependence, as was also noted by Hultgren *et al.*<sup>3</sup>

The boiling point ( $T_{vp}$ ) is 2741.437 K, as calculated as the temperature for which  $\Delta G^o = 0$  for Be(0) = Be(g).

The difference in the enthalpy of vaporization,  $\Delta_{us}H^o = 291.572 \text{ kJ}\cdot\text{mol}^{-1}$ .

**References**

- P. B. Kantor, R. M. Krasovitskaya, and A. N. Kisel, *Fiz. Metal and Metalloved.*, Akad. Nauk SSSR, **10**, 835 (1960).
- E. Baur and R. Brunner, *Helv. Chim. Acta* **17**, 558 (1934).
- R. Hultgren, P. D. Desai *et al.*, "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals, Metals Park, Ohio, 636 pp. (1973).

	T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K	Standard State Pressure = P <sup>o</sup> = 0.1 MPa			
				S <sup>o</sup>	-G <sup>o</sup> -H <sup>o</sup> (T <sub>r</sub> )/T	H <sup>o</sup> -H <sup>o</sup> (T <sub>r</sub> )/T	-Δ <sub>r</sub> H <sup>o</sup>
0	100	0	0	19.539	19.539	0	10.508
	200	16.380	19.540	0.030	15.508	12.478	-2.173
	250	16.472	19.641	0.030	15.508	11.973	-1.287
	300	18.520	22.344	19.749	0.909	15.508	-1.988
	350	19.065	25.917	20.235	1.872	15.508	-1.273
	400	21.061	27.334	20.891	2.899	15.508	10.453
	450	21.943	29.600	21.650	3.975	15.508	10.458
	500	60.0	32.730	22.226	6.242	15.508	9.448
	600	23.236	32.750	23.080	8.654	15.508	-0.330
	700	24.463	31.414	23.080	11.130	15.508	-0.485
	800	25.458	40.746	26.833	13.723	15.508	-0.372
	900	26.384	43.799	28.551	16.406	15.508	6.418
	1000	27.274	46.625	30.219	5.408	15.508	-0.282
	1100	28.147	49.265	31.832	19.177	15.508	-0.209
	1150.000	28.582	50.526	32.617	20.595	GLASS <--> LIQUID	---
	1150.000	27.907	50.526	32.617	20.595	TRANSITION	---
	1200	28.014	51.716	33.388	21.593	15.466	-0.148
	1300	28.229	53.967	34.886	24.805	15.333	-0.096
	1400	28.444	56.067	36.325	27.639	15.134	-0.052
	1500	28.659	58.037	37.707	30.494	14.869	0.427
	1560.000	28.788	59.163	38.511	32.218	BETA <--> LIQUID	---
	1600	28.874	59.893	39.036	33.371	0	0
	1700	29.089	61.050	40.315	36.269	0	0
	1800	29.304	63.319	41.547	39.189	0	0
	1900	29.519	64.509	42.735	42.130	0	0
	2000	29.734	66.429	43.882	45.093	0	0
	2100	29.949	67.884	44.991	48.077	0	0
	2200	30.164	69.283	46.063	51.082	0	0
	2300	30.379	70.628	47.102	54.110	0	0
	2400	30.594	71.926	48.110	57.158	0	0
	2500	30.809	73.179	49.088	60.228	0	0
	2600	31.024	74.391	50.038	63.320	0	0
	2700	31.239	75.566	50.962	66.433	0	0
	2741.437	31.328	76.043	51.317	67.729	FUGACITY = 1 bar	---
	2800	31.454	76.706	51.861	69.588	-29.957	-0.116
	2900	31.669	77.814	52.737	72.724	-289.894	-0.303
	3000	31.884	78.891	53.591	75.901	-288.814	-0.477
	3100	32.099	79.940	54.424	79.101	-287.718	-0.539
	3200	32.314	80.963	55.237	82.321	-286.609	-0.590
	3300	32.529	81.960	56.032	85.563	-285.488	-0.931
	3400	32.744	82.934	56.809	88.827	-284.356	-1.064
	3500	32.959	83.887	57.569	92.112	-283.215	-1.188

CRYSTAL( $\alpha$ - $\beta$ )-LIQUID $A_f = 9.01218$  Beryllium (Be)

0 to 1527 K crystal, alpha  
1527 to 1560 K crystal, beta  
above 1560 K liquid

Refer to the individual tables for details.

$T/K$	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^* = 0.1\text{ MPa}$		
	$C_v^*$	$S^*$ $\text{J K}^{-1}\text{mol}^{-1}$	$H^* - H(T)/T$	$\Delta_H^*$ $\text{kJ mol}^{-1}$	$\Delta_G^*$ $\text{kJ mol}^{-1}$
0	0	0	0	0	0
100	0.1819	0.0503	19.434	-1.932	0
200	0.984	4.174	10.751	-1.151	0
250	13.574	6.801	9.695	-0.723	0
298.15	16.380	9.440	9.440	0	0
300	16.472	9.542	9.440	0.030	0
350	18.520	12.245	9.649	0.909	0
400	19.955	14.817	10.136	1.872	0
450	21.061	17.233	10.792	2.899	0
500	21.943	19.501	11.551	3.975	0
600	23.336	23.630	13.227	6.242	0
700	24.463	27.314	14.981	8.634	0
800	25.458	30.647	16.734	11.130	0
900	26.384	33.699	18.452	13.723	0
1000	27.274	36.523	20.119	16.406	0
1100	28.147	39.166	21.732	19.177	0
1200	29.016	41.652	23.290	22.035	0
1300	29.886	44.069	24.793	24.980	0
1400	30.763	46.256	26.247	28.013	0
1500	31.650	48.409	27.653	31.133	0
1527.000	31.892	48.975	28.025	31.991	$\text{ALPHA} \leftrightarrow \text{BETA}$
1560.000	30.000	53.461	28.025	38.840	TRANSITION
1560.000	30.000	54.102	28.570	39.830	TRANSITION
1560.000	28.788	59.163	28.570	47.725	BETA $\leftrightarrow$ LIQUID
1600	28.874	59.893	29.344	48.879	TRANSITION
1700	29.089	61.650	31.193	51.777	0
1800	29.304	63.319	32.922	54.696	0
1900	29.519	64.909	34.573	57.638	0
2000	29.734	66.429	36.128	60.600	0
2100	29.949	67.884	37.606	63.584	0
2200	30.164	69.283	39.014	66.590	0
2300	30.379	70.628	40.360	69.617	0
2400	30.594	71.926	41.648	72.666	0
2500	30.809	73.129	42.885	75.736	0
2600	31.024	74.391	44.073	78.828	0
2700	31.239	75.566	45.218	81.941	0
2741.437	31.328	76.043	45.680	83.237	FUGACITY = 1 bar
2800	31.454	76.706	46.322	85.075	62.223
2900	31.669	77.814	47.389	88.232	-0.116
3000	31.884	78.891	48.421	91.469	-16.817
3100	32.099	79.940	49.421	94.608	-27.718
3200	32.314	80.963	50.391	97.829	-37.897
3300	32.529	81.960	51.333	101.071	-48.383
3400	32.744	82.934	52.248	104.335	-58.834
3500	32.959	83.887	53.138	107.620	-69.251
					-1.064
					-283.215
					-79.635
					-1.188

PREVIOUS:

CURRENT: September 1983

## Beryllium (Be)

## Beryllium (Be)

## IDEAL GAS

$$\text{IP(Be, g)} = 75192.07 \pm 0.1 \text{ cm}^{-1}$$

$$S^*(298.15 \text{ K}) = 136.274 \pm 0.070 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(0 \text{ K}) = 320 \pm 5 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = 324 \pm 5 \text{ kJ}\cdot\text{mol}^{-1}$$

Electronic Levels and Quantum Weights	
State	$\epsilon_n, \text{cm}^{-1}$
$^1\text{S}_0$	0.0
$^1\text{P}_0$	21978.28
$^3\text{P}_1$	21978.92
$^1\text{P}_1$	21981.27
$^3\text{P}_2$	42565.35
$^1\text{D}_2$	74433.20
$^1\text{P}$	75192.29

## Enthalpy of Formation

The enthalpy of formation is derived from the sublimation studies of Holden *et al.* (1172–1552 K),<sup>1</sup> Gulbranson and Andrew (1103–1229 K),<sup>2</sup> and Hildenbrand and Murad (1400–1500 K).<sup>4</sup> The adopted value,  $\Delta_f H^\circ(\text{Be, g}, 298.15 \text{ K}) = 324 \pm 5 \text{ kJ}\cdot\text{mol}^{-1}$ , is that recommended by CODATA.<sup>5</sup> There are additional vapor pressure studies ( $\sim 20$ ), but they have been omitted in this analysis.

## Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Moore,<sup>6,7</sup> 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 function<sup>8</sup> 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 three levels at  $\sim 22000 \text{ cm}^{-1}$ ; the next excited state is approximately  $42565 \text{ cm}^{-1}$  above the ground state. Since inclusion of these excited states has no effect on the thermodynamic functions (to 6000 K), we list only the ground state. The reported uncertainty in  $S^*(298.15 \text{ K})$  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.<sup>8</sup>

The thermal functions at 298.15 K agree with the CODATA recommendations<sup>5</sup> except that the entropy differs by  $0.1094 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , since this table uses a standard state pressure of 1 bar (CODATA recommendations are based on 1 atm).

## References

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- E. A. Gulbranson and R. F. Andrew, *J. Electrochem. Soc.* **97**, 383 (1950).
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- C. E. Moore, U. S. Nat. Bur. Stand., NSRDS-NBS-35, Volume I, 1970 (Reprint of NBS Circular 467, Volume I, 1949).
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## Be(g) Beryllium (Be)

		Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$					
		$H^\circ - H^\circ(T_0)/T$		$H^\circ - H^\circ(T)/T$		$\Delta_f H^\circ$	
		$C_p^\circ$	$S^\circ$	$-G^\circ - H^\circ(T_0)/T$	$-G^\circ - H^\circ(T)/T$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$
T/K							
0	0.	0.	0.	INFINITE	-6.197	319.735	INFINITE
90	20.786	113.567	154.155	-4.119	323.774	310.468	-76.172
200	20.786	127.975	138.176	-2.040	323.275	298.515	-71.964
250	20.786	132.613	136.617	-1.001	323.723	292.269	-10.066
289.15	20.786	136.274	136.274	0.	324.000	286.184	-50.138
300	20.786	136.403	136.275	0.038	324.008	283.950	-49.788
350	20.786	139.607	136.528	1.078	324.169	279.592	-41.727
400	20.786	142.383	137.090	2.117	324.245	273.218	-35.679
450	20.786	144.831	137.817	3.156	324.257	266.839	-30.974
500	20.786	147.021	138.630	4.196	324.221	260.460	-27.210
600	20.786	150.811	140.354	6.274	324.032	247.724	-21.566
700	20.786	154.015	142.082	8.353	323.719	233.029	-17.538
800	20.786	156.791	143.751	10.431	323.301	222.386	-14.520
900	20.786	159.239	145.339	12.510	320.802	212.177	-10.305
1000	20.786	161.429	146.840	14.589	322.183	197.279	-10.305
1100	20.786	163.410	148.253	16.667	321.490	184.822	-8.776
1200	20.786	165.219	149.597	18.746	320.711	172.431	-7.506
1300	20.786	166.882	150.863	20.824	319.844	160.109	-6.433
1400	20.786	168.423	152.063	22.903	318.890	147.857	-4.717
1500	20.786	169.857	152.000	24.982	317.848	133.676	-4.717
1600	20.786	171.198	154.286	27.060	302.182	124.093	-4.051
1700	20.786	171.428	155.183	29.159	301.362	112.988	-3.472
1800	20.786	173.647	156.303	31.218	300.521	101.931	-2.938
1900	20.786	174.770	157.246	33.296	299.659	90.922	-2.500
2000	20.786	175.837	158.149	35.375	298.775	79.958	-2.088
2100	20.791	176.851	159.016	37.454	297.870	69.040	-1.717
2200	20.795	177.818	159.846	39.533	296.943	58.165	-1.381
2300	20.801	178.743	160.650	41.613	295.996	47.232	-1.075
2400	20.811	179.628	161.422	43.694	295.028	36.541	-0.795
2500	20.824	180.478	162.168	45.775	294.039	25.791	-0.539
2600	20.844	181.295	162.888	47.859	293.031	15.081	-0.303
2700	20.850	182.082	163.584	49.934	292.003	4.410	-0.085
2741.437	20.883	182.400	163.867	50.809	— FUGACITY = 1 bar —		
2800	20.905	182.842	164.259	52.033	— FUGACITY = 1 bar —		
3000	21.006	184.287	165.546	56.223	— FUGACITY = 1 bar —		
3100	21.075	184.977	166.162	58.327	— FUGACITY = 1 bar —		
3200	21.159	185.648	166.761	60.439	— FUGACITY = 1 bar —		
3300	21.259	186.300	167.343	62.559	— FUGACITY = 1 bar —		
3400	21.376	186.937	167.910	64.691	— FUGACITY = 1 bar —		
3500	21.512	187.558	168.465	66.835	— FUGACITY = 1 bar —		
3600	21.668	188.184	168.762	169.527	— FUGACITY = 1 bar —		
3700	21.844	188.792	169.001	169.994	— FUGACITY = 1 bar —		
3800	22.041	189.347	170.044	170.544	— FUGACITY = 1 bar —		
3900	22.259	189.923	171.035	171.816	— FUGACITY = 1 bar —		
4000	22.500	190.489	171.048	172.516	— FUGACITY = 1 bar —		
4100	22.761	191.048	171.516	180.079	— FUGACITY = 1 bar —		
4200	23.045	191.600	171.988	182.569	— FUGACITY = 1 bar —		
4300	23.349	192.146	172.451	187.639	— FUGACITY = 1 bar —		
4400	23.674	192.686	172.904	187.040	— FUGACITY = 1 bar —		
4500	24.019	193.222	173.350	189.424	— FUGACITY = 1 bar —		
5100	26.443	196.371	175.874	194.544	— FUGACITY = 1 bar —		
5200	26.894	196.889	176.223	197.944	— FUGACITY = 1 bar —		
5300	27.334	197.405	176.688	194.282	— FUGACITY = 1 bar —		
5400	27.822	197.921	177.036	192.673	— FUGACITY = 1 bar —		
4800	24.764	194.808	174.642	196.798	— FUGACITY = 1 bar —		
4900	25.162	195.331	175.058	197.459	— FUGACITY = 1 bar —		
5000	26.003	195.832	175.469	191.913	— FUGACITY = 1 bar —		
5100	26.443	196.371	175.874	194.544	— FUGACITY = 1 bar —		
5200	26.894	196.889	176.223	197.944	— FUGACITY = 1 bar —		
5300	27.334	197.405	176.688	194.282	— FUGACITY = 1 bar —		
5400	27.822	197.921	177.036	192.673	— FUGACITY = 1 bar —		
5500	28.296	198.436	177.446	195.479	— FUGACITY = 1 bar —		
5600	28.776	198.950	177.819	198.333	— FUGACITY = 1 bar —		
5700	29.258	199.464	178.195	201.234	— FUGACITY = 1 bar —		
5800	29.743	199.977	178.566	202.185	— FUGACITY = 1 bar —		
5900	30.227	200.489	178.933	203.183	— FUGACITY = 1 bar —		
6000	30.711	201.001	179.296	203.230	— FUGACITY = 1 bar —		

PREVIOUS: September 1961 (1 atm)  
CURRENT: September 1983 (1 bar)

Beryllium (Be)

$M_f = 9.01163$  Beryllium, Ion ( $\text{Be}^+$ )

IDEAL GAS

$$\begin{aligned}P(\text{Be}^+, g) &= 146882.86 \pm 0.1 \text{ cm}^{-1} \\S^\circ(298.15 \text{ K}) &= 142.037 \pm 0.02 \text{ J K}^{-1} \cdot \text{mol}^{-1}\end{aligned}$$

$$\Delta_f^{\text{H}}(0\text{ K}) = 1208.77 \pm 5.0 \text{ kJ/mol}^{-1}$$

$$\Delta_f^{\text{H}}(700\text{ K}) = (1210.321 \pm 0.001) \text{ kJ/mol}^{-1}$$

Electronic Levels and Quantum Weights	
State	$\epsilon_i, \text{cm}^{-1}$
$S_0$	0.0
$S_1$	31928.8
$S_2$	31935.4

Enthalpy of Formation

$\Delta H_f^\circ(\text{Be}^*, \text{g}, 0 \text{ K})$  is calculated from  $\Delta h_f^\circ(\text{Be}, \text{g}, 0 \text{ K})$  using the spectroscopic value of IP(Be) with JANAF<sup>1</sup> enthalpy of formation data. The ionization limit is converted from  $\text{cm}^{-1}$  to  $\text{kJ}\cdot\text{mol}^{-1}$  using the factor derived from the 1973 CODATA fundamental constants.<sup>2</sup> Rossenstock *et al.*<sup>3</sup> and Levin and Lias<sup>4</sup> appearance potential data.

$\Delta H_f^\circ(\text{Be}^*, \text{g}, 298.15 \text{ K})$  is calculated from  $\Delta h_f^\circ(\text{Be}, \text{g}, 0 \text{ K})$  by using IP(Be) with JANAF<sup>1</sup> enthalpy of formation data, Be<sup>(g)</sup>, and e<sup>(ref.)</sup>.  $\Delta H_f^\circ(\text{Be} \rightarrow \text{Be}^* \text{e}^-, 298.15 \text{ K})$  differs from a room temperature threshold energy to threshold effects discussed by Rossenstock *et al.*<sup>3</sup>  $\Delta H_f^\circ(298.15 \text{ K})$  should be changed by  $-6.1$  eV to exclude the enthalpy of the electron convention that excludes the enthalpy of the electron.

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**Heat Capacity and Entropy**  
The information on electronic energy levels and quantum weights, given by Moore,<sup>2,6</sup> 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 function<sup>7</sup> 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 88231.2 cm<sup>-1</sup> above the ground state and the first two excited states. The reported uncertainty in  $S^{\infty}(298.15\text{ K})$  is due to uncertainties in the relative ionic mass and the fundamental constants.

- References**

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**Enthalpy of Formation**  $\Delta H^\circ(\text{Be}, 0 \text{ K})$  is calculated from  $\Delta H^\circ(\text{Be, g, } 0 \text{ K})$  using the spectroscopic value of  $\text{IP}(\text{Be}) = 75192.07 \pm 0.1 \text{ cm}^{-1}$  ( $899.497 \pm 0.001 \text{ kJ mol}^{-1}$ ) from Moore.<sup>2</sup> The ionization limit is converted from  $\text{cm}^{-1}$  to  $\text{kJ mol}^{-1}$  using the factor,  $1 \text{ cm}^{-1} = 0.0119266 \text{ kJ mol}^{-1}$ , which is derived from the 1973 CODATA fundamental constants. Rosensweig<sup>3</sup> and Levin<sup>4</sup> have summarized additional contributions.

threshold effects discussed by Rosentock *et al.*<sup>4</sup>  $\Delta H^\circ(298.15\text{ K})$  should be changed by  $-6.197 \text{ kJ}\cdot\text{mol}^{-1}$  if it is to be used in the ion conversion that excludes the enthalpy of the electron appearance potential data.

**Enthalpy of Formation**  $\Delta H^\circ_f(R^{\bullet}, 0^\circ K)$  is calculated from  $\Delta H^\circ_f(R, 0^\circ K)$  using the recommended values of  $\Delta H^\circ_f$ .

$\Delta H^\circ$  (Be<sup>+</sup>, g, 298.15 K) is calculated from  $\Delta fH^\circ$  (Be<sup>+</sup>, g, 0 K) by using IP(Be) with JANAF<sup>1</sup> enthalpies,  $H^\circ$ (0 K)- $H^\circ$ (298.15 K), for Be<sup>+</sup> (e.g., Be<sup>+</sup>(g), and e<sup>-</sup>(ref)).  $\Delta H^\circ$ (Be<sup>+</sup>Be<sup>+</sup>e<sup>-</sup>, 298.15 K) differs from a room temperature threshold energy due to inclusion of these enthalpies and no threshold effect discussed by Rossenstock *et al.*<sup>4</sup>  $\Delta H^\circ$ (298.15 K) should be changed by  $-6.197 \text{ kJ}\cdot\text{mol}^{-1}$  if it is to be used in the ionization convention that excludes the enthalpy of the electron.

Enthalpy/Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$		
$T/\text{K}$	$C_p^{\circ}/\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$H^\circ - H^\circ(T_r)/\text{J}\cdot\text{T}$	$\Delta H^\circ/\text{kJ}\cdot\text{mol}^{-1}$	$\Delta G^\circ/\text{kJ}\cdot\text{mol}^{-1}$
0	0	0	-6.197	1208.770
100	20.786	119.330	-4.119	
200	20.786	133.737	-2.904	
250	20.786	138.376	-1.001	
298.15	142.037	142.037	0.	1219.232
300	20.786	145.370	-1.250	
350	20.786	148.155	-0.708	
400	20.786	148.593	-2.052	
500	20.786	152.783	-1.392	
600	20.786	156.573	-1.116	
700	20.786	174.777	-1.473	
800	20.786	162.553	-1.514	
900	20.786	165.000	-1.011	
1000	20.786	167.191	-1.502	
1100	20.786	169.170	-1.420	
1200	20.786	170.981	-1.559	
1300	20.786	174.815	-1.626	
1400	20.786	174.185	-1.526	
1500	20.786	175.619	-1.865	
1600	20.786	176.261	-1.048	
1700	20.786	178.221	-1.080	
1800	20.786	179.409	-1.066	
1900	20.786	180.533	-1.030	
2000	20.786	181.599	-1.012	
2100	20.786	182.613	-1.044	
2200	20.786	183.580	-1.011	
2300	20.786	184.504	-1.412	
2400	20.786	185.389	-1.185	
2500	20.786	186.237	-1.930	
2600	20.786	187.052	-1.786	
2700	20.786	187.786	-1.246	
2800	20.787	188.593	-0.020	
2900	20.787	189.327	-1.073	
3000	20.787	190.027	-1.307	
3100	20.788	190.709	-1.729	
3200	20.788	191.369	-1.719	
3300	20.790	192.008	-1.665	
3400	20.792	192.629	-1.705	
3500	20.795	193.232	-1.416	
3600	20.798	193.818	-1.752	
3700	20.802	194.388	-1.725	
3800	20.806	194.942	-1.785	
3900	20.812	195.483	-1.684	
4000	20.820	196.010	-1.770	
4100	20.829	196.524	-1.246	
4200	20.839	197.026	-1.711	
4300	20.851	197.517	-1.886	
4400	20.865	197.966	-1.611	
4500	20.882	198.465	-1.947	
4600	20.900	198.924	-1.374	
4700	20.921	199.374	-1.983	
4800	20.945	199.815	-1.803	
4900	20.972	200.247	-1.804	
5000	20.971	200.671	-2.047	
5100	21.033	181.489	-1.801	
5200	21.069	181.870	-1.057	
5300	21.108	182.244	-1.046	
5400	21.150	182.992	-1.811	
5500	21.195	182.973	-2.023	
5600	21.244	203.063	-183.328	
5700	21.297	203.479	-183.678	
5800	21.353	203.811	-184.022	
5900	21.412	204.176	-184.360	
6000	21.475	204.537	-184.693	

Beryllium Ion ( $\text{Be}^+$ )

CURRENT: September 1983 (1 bar)

**Be<sub>2</sub>Br<sub>4</sub>(g)****M<sub>r</sub> = 88.91618 Beryllium Bromide (BeBr)****IDEAL GAS**

$$\Delta H^\circ(0\text{ K}) = 125.3 \pm 41.8 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(298.15\text{ K}) = [228.5 \pm 0.4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

State	$\epsilon, \text{cm}^{-1}$	g <sub>e</sub>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K			Standard State Pressure = p <sup>o</sup> = 0.1 MPa		
			T/K	C <sub>p</sub> <sup>o</sup> /J K <sup>-1</sup> mol <sup>-1</sup>	S <sup>o</sup> /J K <sup>-1</sup> mol <sup>-1</sup>	-[G <sup>o</sup> - H <sup>o</sup> (T)]/T/kJ mol <sup>-1</sup>	H <sup>o</sup> - H <sup>o</sup> (T)/kJ mol <sup>-1</sup>	
X <sub>2</sub> <sup>+</sup>	0	2	0	0	0	INFINITE	-8.971	125.326
A <sub>1</sub> T <sub>1g</sub>	26353.2	2	100	29.145	195.462	-6.063	126.799	109.995
A <sub>1</sub> T <sub>1g</sub>	26550.2	2	200	30.486	215.960	-231.450	126.735	-57.455
B <sub>1</sub> [2]	[27000]	[2]	250	31.597	222.881	-229.065	-1.546	-23.320
C[1]	[40000]	[4]	298.15	32.598	228.334	228.534	0	120.110
			300	32.633	228.736	228.535	0.060	120.070
			350	33.508	233.834	228.935	1.021	70.926
			400	34.218	238.357	229.836	3.408	104.336
			450	34.787	242.421	231.012	5.134	104.114
			500	35.246	246.111	232.340	6.3817	61.377
			600	35.922	252.601	235.191	10.446	56.642
			700	36.386	258.175	238.086	14.063	102.654
			800	36.721	263.057	240.908	17.719	101.938
			900	36.973	267.397	243.615	21.404	101.148
			1000	37.170	271.303	246.192	25.112	100.634
$\omega_e = 715.06 \text{ cm}^{-1}$	$\omega_e c_e = 4.30 \text{ cm}^{-1}$	$\sigma = 1$						-0.082
$B_e = [0.621551] \text{ cm}^{-1}$	$\alpha_e = [0.0052851] \text{ cm}^{-1}$	$r_e = [1.83] \text{ \AA}$						

**Enthalpy of Formation**

No thermochemical measurement of the enthalpy of formation has been made. The selected value,  $\Delta_H^\circ(\text{BeBr}, g, 0\text{ K}) = 30.0 \pm 10.0 \text{ kcal}\cdot\text{mol}^{-1}$ , is obtained from an analysis of spectroscopic data. The adopted values for the ground state vibrational constants give  $D_0^\circ = 3.64 \text{ eV}$  by a linear Birge-Sponer extrapolation.<sup>1</sup> Based on the ionicity correction developed by Hildenbrand,<sup>2</sup> this value adjusts to  $D_0^\circ = 3.271 \text{ eV}$  ( $75.46 \text{ kcal}\cdot\text{mol}^{-1}$ ) which is adopted.  $\Delta_H^\circ(298.15 \text{ K})$  corresponds to  $28.7 \text{ kcal}\cdot\text{mol}^{-1}$ . Ionic model calculations<sup>3,4</sup> and bond energy correlations<sup>5</sup> have led to  $D_0^\circ$  values of (in eV) 1.2,<sup>4</sup> 1,<sup>5</sup> and 2.1.<sup>6</sup> The latter value which is based on a Rittner potential<sup>7</sup> is believed to represent a minimum value for  $D_0^\circ$ . Additional support for the adopted value of  $\Delta_H^\circ$  is provided by a comparison of values for the ratio  $D_0^\circ(\text{MX}, 298.15 \text{ K})/\Delta_m H^\circ(\text{MX}, 298.15 \text{ K})$  for the alkaline-earth halides. We find  $D_0^\circ(\text{BeBr}, 298.15 \text{ K})/\Delta_m H^\circ(\text{BeBr}_2, 298.15 \text{ K}) = 0.41$  which is quite consistent with values of this ratio for other alkaline-earth halides.

**Heat Capacity and Entropy**

We estimate  $r_e$  to be 0.08 Å, less than that for BeBr<sub>2</sub>.<sup>3</sup> This estimation is made based on the observation that the ratio  $r_e(\text{MXY})/r_e(\text{MX})$  is near 0.96 for several alkaline-earth halides.<sup>3</sup> The value of  $B_e$  is calculated from  $r_e$ . The value of  $B_e$  is obtained from the other constants by assuming a Morse potential function.

The ground state vibrational constants are taken from the results of a recent vibrational analysis of the A<sup>2</sup>Π-X<sup>Σ</sup> system by Reddy *et al.*<sup>8</sup> Other values<sup>9</sup> for these constants are slightly different than ours, but we consider them to be less accurate. It should also be noted that the values for  $\omega_e c_e$  tabulated by Rosen<sup>9</sup> for the ground and first excited states have been inadvertently reversed. The electronic level for the A<sub>1</sub>T<sub>1g</sub> state is also taken from Reddy *et al.*<sup>8</sup> The doublet splitting of this state is assumed to be 197 cm<sup>-1</sup> as was observed in the emission spectrum of BeBr by Reddy and Rao.<sup>10</sup> We also include a C<sup>2</sup>Π level at 27000 cm<sup>-1</sup> and a C<sup>2</sup>Π level at 40000 cm<sup>-1</sup>. These levels are estimated by analogy with those for CaBr, SrBr, and BaBr.<sup>11</sup>

**References**

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## Beryllium Bromide (BeBr<sub>2</sub>)

## IDEAL GAS

## M<sub>r</sub> = 168.82018 Beryllium Bromide (BeBr<sub>2</sub>)

## Be<sub>1</sub>Br<sub>2</sub>(g)

$$S^o(298.15 \text{ K}) = [273.9 \pm 2.1] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_fH^o(0 \text{ K}) = [-215.8 \pm 16.7] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_fH^o(298.15 \text{ K}) = [-229.3 \pm 16.7] \text{ kJ}\cdot\text{mol}^{-1}$$

Vibrational Frequencies and Degeneracies

$\nu, \text{cm}^{-1}$	No. of Points	T/K	$C_p^o$	$S^o$	$-C_v^o - H(T)/T$	$H^o - H(T_r)$	$\Delta H^o$	$\log K_t$
227 (1)	0	0	0	0	INFINITE	-12.917	-215.758	INFINITE
220 (2)	100	40.423	22.1826	318.498	-9.667	-215.341	-232.089	121.231
1010 (1)	200	49.650	253.339	278.580	-5.068	-216.221	-248.570	64.920
	250	51.746	264.655	274.778	-2.531	-217.091	-256.564	53.606
	298.15	53.315	273.909	273.909	0.	-229.283	-262.754	46.033

Ground State Quantum Weight: [1]

$\sigma = 2$

Point Group: D<sub>∞h</sub>

Bond Distance: Be-Br = 1.91 ± 0.02 Å

Bond Angle: Br-Br-Br = 180°

Rotational Constant:  $B_o = [0.028916] \text{ cm}^{-1}$

## Enthalpy of Formation

Rahils and Fischer<sup>1</sup> have reported measurements of the sublimation pressures (624–655 K) and vapor densities (736–799 K) for BeBr<sub>2</sub>. Both measurements were complicated by significant reaction of the dibromide with the quartz apparatus. Assuming the reaction to be 2BeBr<sub>2</sub>(cr) + SiO<sub>2</sub>(cr) = SiBr<sub>4</sub>(g) + 2BeO<sub>cr</sub>, Rahils and Fischer<sup>1</sup> corrected their measured total pressure for the partial pressure of the tetrabromide. Results of a 2nd and 3rd law analyses of their data are tabulated below.

No. of Points	$\Delta_{abs}H^o(298.15 \text{ K}), \text{ kcal/mol}^{-1}$	Drift, $\Delta H^o(298.15 \text{ K})$ , kcal/mol <sup>-1</sup>	$\Delta H^o(298.15 \text{ K})$ , kcal/mol <sup>-1</sup>
Sublimation Pressures <sup>a</sup>	624–605	31.0	30.2 ± 0.1
Vapor Densities—	736–799	23.9	33.4 ± 1.0
Total Pressures <sup>b</sup>			-1.0 ± 0.8
			12.4 ± 9.0
			-54.8
			-51.6

\*Pressures assigned to monomer. \*One point rejected due to failure of a statistical test. \*Pressures corrected for dimer.

The vapor density measurements<sup>1</sup> predict about 50% dimerization at temperatures near the melting point ( $T_m = 781 \text{ K}$ ). This value appears to be unusually high when compared with dimerization data which are available for BeCl<sub>2</sub>, MgBr<sub>2</sub>, MgCl<sub>2</sub>, and MgF<sub>2</sub>.<sup>2</sup> Mass spectral studies of these alkaline-earth dihalides show the presence of only small amounts (1–5%) of dimer in the saturated vapors up to temperatures near their melting points. Electron-diffraction experiments on BeBr<sub>2</sub> vapor are also inconsistent with high concentrations of dimer. It is quite likely that the monomer and dimer pressures reported by Rahils and Fischer<sup>1</sup> from their vapor density measurements are unreliable. Thus, we choose to adopt  $\Delta_fH^o(298.15 \text{ K}) = -54.8 \text{ kcal/mol}^{-1}$  rather than the average value ( $-53.2 \text{ kcal/mol}^{-1}$ ) of these two results. The sublimation pressures<sup>c</sup> are assigned solely to the monomer pending resolution of the dimerization problem. Also,  $\Delta_fH^o(\text{gr})$  is placed in brackets to emphasize the uncertainties in  $\Delta_fH^o(\text{gr})$ .

## Heat Capacity and Entropy

Information available on the structure of BeBr<sub>2</sub> tend to indicate that the molecule is linear. Electron-diffraction patterns<sup>3,4</sup> for BeBr<sub>2</sub> vapor have been successfully interpreted in terms of a linear configuration. Buchlier *et al.*<sup>5</sup> using electric quadrupole deflection of molecular beams to detect permanent dipole moments in molecules, have shown that for the gaseous alkaline-earth dihalides the linear form is favored by a light metal-heavy halogen combination. The matrix-isolation spectrum<sup>6</sup> of BeBr<sub>2</sub> shows the two infrared-active vibrations which would be expected for a linear molecule. We adopt the linear configuration. The bond length is taken from the electron-diffraction studies of Akishin,<sup>3,4</sup> and the asymmetric stretching ( $\nu_3$ ) and bending ( $\nu_2$ ) frequencies have been observed in the matrix-isolation spectrum of BeBr by Snelson.<sup>6</sup> The adopted frequencies are gas-phase values which were estimated by Snelson<sup>6</sup> from the matrix data. The infrared-inactive symmetric stretching frequency ( $\nu_1$ ) is calculated from an estimated force constant by a simple valence force field approximation.<sup>7</sup> The stretching force constant ( $K = 2.430 \times 10^5 \text{ dynes/cm}$ ) is assumed equal to that for BeBr. Literature estimates of  $\nu_1$  include (in  $\text{cm}^{-1}$ ) 230<sup>8,9</sup> and 209.<sup>9</sup> The ground state quantum weight of one is assigned by analogy with BaCl<sub>2</sub>.<sup>2</sup> Brewer *et al.*<sup>8</sup> have tabulated Gibbs energy functions for BeBr up to 1500 K. Their values are consistently lower than ours by about 2.5 cal/K<sup>-1</sup>·mol<sup>-1</sup>. These differences are due entirely to the higher bending frequency ( $\nu_2 = 446 \text{ cm}^{-1}$ ) which was used by Brewer *et al.*<sup>8</sup> This estimated value is now known to be incorrect.

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- JANAF Thermochemical Tables: Be<sub>2</sub>Cl<sub>4</sub>(g), 6–30–65; Mg<sub>2</sub>Cl<sub>4</sub>(g), 12–31–66; Mg<sub>2</sub>Br<sub>4</sub>(g), 6–30–75; BeBr(g), 6–30–75; BaCl<sub>2</sub>(g), 12–31–72.

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Beryllium Bromide (BeBr <sub>2</sub> )								
Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$				Standard State Pressure = $P^o = 0.1 \text{ MPa}$				CURRENT June 1975 (1 bar)
$T/K$	$C_p^o$	$S^o$	$-C_v^o - H(T)/T$	$H^o - H(T_r)$	$\Delta H^o$	$\log K_t$		
0	0	0	INFINITE	-12.917	-215.758	INFINITE		
100	40.423	22.1826	318.498	-9.667	-215.341	-232.089	121.231	
200	49.650	253.339	278.580	-5.068	-216.221	-248.570	64.920	
250	51.746	264.655	274.778	-2.531	-217.091	-256.564	53.606	
298.15	53.315	273.909	273.909	0.	-229.283	-262.754	46.033	
300	53.369	274.239	273.910	0.099	-229.335	-262.962	45.786	
350	54.705	282.369	274.364	280.02	-260.180	-266.871	39.828	
400	55.816	289.949	276.035	5.563	-260.210	-267.826	34.974	
450	56.740	296.578	277.955	8.380	-260.264	-268.74	31.199	
500	57.507	302.597	280.123	11.237	-260.333	-269.716	14.556	
600	58.673	313.191	284.776	17.049	-260.507	-271.578	23.643	
700	59.490	322.301	289.501	22.960	-260.726	-273.406	20.402	
800	60.075	330.285	294.110	28.940	-260.996	-275.406	17.969	
900	60.504	337.387	298.531	34.970	-261.322	-276.956	16.074	
1000	60.826	343.779	302.742	41.037	-261.712	-278.673	14.556	
1100	61.072	349.588	306.741	47.132	-262.171	-280.347	13.313	
1200	61.265	354.911	310.536	53.250	-262.704	-281.970	12.274	
1300	61.418	359.821	314.141	59.384	-263.330	-283.559	11.394	
1400	61.543	364.377	317.568	65.532	-264.009	-284.091	10.637	
1500	61.643	368.627	320.832	71.692	-264.789	-285.570	9.979	
1600	61.726	372.608	322.945	77.860	-280.195	-287.468	9.385	
1700	61.796	376.552	326.937	84.037	-281.396	-287.906	8.846	
1800	61.855	379.886	329.764	90.219	-281.348	-288.309	8.367	
1900	61.906	383.232	332.491	96.407	-281.970	-288.679	7.936	
2000	61.949	386.408	335.108	102.600	-282.636	-289.015	7.548	
2100	61.986	389.432	337.624	108.797	-283.317	-289.318	7.196	
2200	62.018	392.316	340.045	114.997	-284.047	-289.587	6.876	
2300	62.047	395.073	342.378	121.200	-284.816	-289.822	6.582	
2400	62.072	397.715	344.629	127.406	-285.626	-290.022	6.312	
2500	62.094	402.249	346.803	133.615	-286.478	-290.188	6.063	
2600	62.114	402.685	348.906	139.825	-287.372	-290.339	5.833	
2700	62.131	407.029	350.944	146.037	-288.307	-290.414	5.618	
2800	62.147	407.729	352.914	152.251	-289.243	-291.457	5.203	
2900	62.161	409.470	354.827	158.467	-289.198	-291.527	4.930	
3000	62.174	411.578	356.883	164.683	-290.174	-293.113	4.581	
3100	62.185	413.617	358.487	170.901	-290.171	-292.544	4.255	
3200	62.196	415.591	360.241	183.341	-290.189	-294.197	3.950	
3300	62.205	417.505	361.947	193.549	-290.207	-294.406	3.663	
3400	62.214	419.362	363.609	195.562	-290.284	-294.835	3.393	
3500	62.222	421.166	365.228	195.783	-290.359	-295.222	3.138	
3600	62.230	422.919	366.906	202.006	-290.451	-299.686	2.897	
3700	62.236	424.624	368.346	204.279	-290.560	-299.108	2.670	
3800	62.243	426.284	369.949	214.433	-290.685	-298.526	2.454	
3900	62.249	427.901	371.317	220.678	-290.826	-297.942	2.249	
4000	62.254	429.477	372.551	226.903	-290.983	-297.533	2.035	
4100	62.259	431.014	374.153	233.129	-291.156	-298.170	1.870	
4200	62.264	432.514	375.525	239.325	-291.345	-298.379	1.693	
4300	62.268	433.979	376.968	245.581	-291.530	-298.526	1.525	
4400	62.272	435.441	378.182	251.808	-291.772	-298.736	1.365	
4500	62.276	436.810	379.469	258.036	-292.012	-299.270	1.211	
4600	62.279	438.179	380.731	264.263	-292.270	-299.724	1.064	
4700	62.283	439.519	381.967	270.491	-292.547	-300.100	0.924	
4800	62.286	440.830	382.524	276.720	-292.843	-302.471	0.789	
4900	62.289	442.114	384.270	282.949	-293.160	-303.835	0.659	
5000	62.291	443.373	385.537	283.188	-293.489	-304.355	0.535	
5100	62.294	444.606	386.683	295.407	-293.859	-305.542	0.415	
5200	62.296	445.816	387.809	301.636	-294.242	-306.270	0.300	
5300	62.299	447.003	388.915	307.866	-294.659	-307.220	0.189	
5400	62.301	448.167	390.001	314.056	-295.081	-308.548	0.083	
5500	62.303	449.310	391.069	320.326	-295.482	-313.3	-0.020	
5600	62.305	450.433	392.119	326.557	-296.019	-312.822	-0.120	
5700	62.307	451.536	393.152	322.787	-296.528	-312.520	-0.216	
5800	62.308	452.619	394.168	329.018	-297.062	-313.227	-0.300	
5900	62.310	453.684	395.188	343.229	-297.688	-314.227	-0.398	
6000	62.312	454.732	396.152	351.480	-298.213	-315.670	-0.483	

Beryllium Bromide (BeBr <sub>2</sub> )								
Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$								

Be<sub>2</sub>Cl<sub>4</sub>(g)

$$M_r = 44.46518 \text{ Beryllium Chloride (BeCl)}$$

$\Delta_f H^\circ(0\text{ K}) = 58.3 \pm 12.6 \text{ kJ}\cdot\text{mol}^{-1}$		$S^\circ(298.15\text{ K}) = [217.6] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$		Reference Temperature = $T_r = 298.15\text{ K}$				Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$			
				$C_p^\circ$		$S^\circ - [G^\circ - H^\circ(T_r)]/T$		$H^\circ - H^\circ(T_r)/T$		$\Delta_f G^\circ$	
				0	0	INFINITE	-8.860	58.331	58.331	0	log K <sub>r</sub>
State	$\epsilon_\infty, \text{cm}^{-1}$	$\delta_1$		100	29.118	195.044	244.558	59.743	50.739	-26.504	
X <sup>2+</sup>	0	2		200	29.867	205.369	220.449	60.383	41.340	-10.797	
A <sup>2</sup>	27970	4		250	30.735	212.124	218.131	60.696	36.513	-7.629	
$\omega_e = 845.29 \text{ cm}^{-1}$	$\omega_{e\infty} = 4.831 \text{ cm}^{-1}$	$\sigma = 1$		298.15	31.642	217.615	217.615	0	60.668	31.856	-5.581
$B_e = [0.769] \text{ cm}^{-1}$	$\alpha_e = [0.0063] \text{ cm}^{-1}$	$r_e = [1.75] \text{ \AA}$		300	31.677	217.811	217.615	0.059	60.665	31.677	-5.516
				350	32.554	222.761	218.004	1.665	60.533	26.856	-40.008
				400	33.316	227.159	218.879	3.121	60.141	22.057	-2.880
				450	33.957	231.121	220.023	4.994	60.109	17.235	-2.006
				500	34.490	241.727	221.315	6.705	59.847	12.541	-1.310
				600	35.301	241.092	224.095	10.198	59.256	3.134	-0.273
				700	35.872	251.397	229.688	13.758	58.89	-6.168	
				800	36.285	255.690	232.343	21.012	57.851	-15.370	1.004
				900	36.596	265.826	234.857	24.684	56.164	-33.486	-24.475
				1000	36.836	269.536	238.729	27.287	55.211	-42.405	0.660
				1100	37.029	263.079	237.281	32.089	54.183	-51.235	2.014
				1200	37.187	266.308	239.567	32.089	53.077	-59.975	2.210
				1300	37.319	269.589	241.700	35.814	51.892	-68.627	2.561
				1400	37.443	272.039	243.808	39.555	50.524	-71.192	2.688
				1500	37.533	274.646	245.749	43.300	50.524	-71.192	
				1600	37.622	277.071	247.659	47.058	43.37	-85.144	2.780
				1700	37.702	279.354	249.457	50.824	33.100	-92.605	2.845
				1800	37.776	281.511	251.179	54.958	32.446	-100.004	2.902
				1900	37.844	283.555	252.839	58.779	31.572	-107.345	2.951
				2000	37.908	285.498	254.415	62.167	31.478	-114.628	2.994
				2100	37.968	287.349	255.929	65.96	29.364	-121.836	3.031
				2200	38.025	289.117	257.407	69.760	28.228	-129.030	3.064
				2300	38.080	290.808	258.823	73.565	27.069	-136.152	
				2400	38.133	292.430	260.190	77.736	25.886	-143.224	3.117
				2500	38.184	293.988	261.511	81.192	24.680	30.245	3.139
				2600	38.233	295.486	262.799	85.013	23.448	-157.218	3.159
				2700	38.292	296.930	264.027	88.839	22.190	-164.143	3.176
				2800	38.329	298.323	265.227	92.669	20.953	-170.050	3.201
				2900	38.376	299.669	266.392	96.503	20.503	-161.035	
				3000	38.423	300.971	267.523	100.345	19.345	-157.263	2.738
				3100	38.469	302.232	268.622	104.189	20.821	-153.482	
				3200	38.515	303.434	269.672	108.038	21.101	-149.693	2.843
				3300	38.562	304.639	271.174	111.892	20.318	-145.894	2.309
				3400	38.609	305.791	271.747	115.751	21.704	-142.087	2.183
				3500	38.656	306.911	272.726	119.614	22.707	-138.270	
				3600	38.705	308.001	273.700	123.482	22.268	-134.443	
				3700	38.754	309.062	274.642	127.152	22.776	-130.607	1.844
				3800	38.803	310.096	275.561	131.233	22.101	-126.761	1.742
				3900	38.857	311.105	276.460	135.116	22.345	-122.905	1.646
				4000	38.911	312.089	277.338	139.004	22.599	-119.038	1.554
				4100	38.967	313.051	278.198	142.988	22.343	-115.161	1.467
				4200	39.025	313.991	279.039	146.798	22.002	-117.273	1.384
				4300	39.083	314.910	279.862	150.703	21.726	-117.276	
				4400	39.148	315.809	280.669	154.615	21.555	-103.464	0.833
				4500	39.212	316.689	281.460	158.533	21.296	-99.542	1.155
				4600	39.280	317.532	282.458	162.458	21.034	-91.608	1.019
				47000	39.350	318.397	282.935	166.389	20.7410	-91.662	1.019
				48000	39.423	319.227	283.742	170.726	20.002	-87.704	
				49000	39.490	320.040	284.474	174.724	20.744	-83.733	0.954
				50000	39.578	320.839	285.193	178.228	20.261	-79.749	
				51000	39.660	321.624	285.920	182.190	20.646	-75.752	0.776
				52000	39.745	322.130	286.595	186.160	20.848	-72.721	0.771
				53000	39.833	323.152	287.277	190.139	21.134	-67.719	0.667
				54000	39.923	323.898	287.948	194.125	20.820	-63.681	0.516
				55000	40.017	324.631	288.609	198.123	20.284	-59.630	0.366
				56000	40.114	325.353	289.238	202.130	20.446	-283.631	0.518
				57000	40.213	326.064	289.885	206.446	20.844	-284.446	0.472
				58000	40.316	326.764	290.528	210.173	20.528	-285.285	0.427
				59000	40.421	327.454	291.148	214.210	20.281	-285.147	0.383
				60000	40.529	328.135	291.738	218.257	20.064	-287.013	0.341

## **Beryllium Chloride ( $\text{BeCl}_2$ )**

## NIST-JANAF THERMOCHEMICAL TABLES

Beryllium Chloride, Ion (BeCl<sup>+</sup>)

## IDEAL GAS

$$\Delta H^{\circ}(0\text{ K}) = [970 \pm 84] \text{ J}\cdot\text{mol}^{-1}$$

$$\Delta H^{\circ}(298.15\text{ K}) = [979 \pm 84] \text{ kJ}\cdot\text{mol}^{-1}$$

$$S^{\circ}(298.15\text{ K}) = [213.0 \pm 8] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

State	Electronic Levels and Quantum Weights $\epsilon_{\nu}$ , cm <sup>-1</sup>	$g_i$
$ \Sigma^+_{1g}\rangle$	0	1
$ \Pi^+_{1g}\rangle$	[10000]	6
$ \Pi^+_{1u}\rangle$	[15000]	2
$ \Sigma^+_{1u}\rangle$	[30000]	3
$ \Delta^+\rangle$	[35000]	2
$ \Sigma^+_{2s}\rangle$	[40000]	1

$$\omega_e = [700] \text{ cm}^{-1}$$

$$\omega_{e\epsilon} = [4.8] \text{ cm}^{-1}$$

$$\sigma = 1$$

$$r_c = [1.8] \text{ \AA}$$

$$B_e = [0.7241] \text{ cm}^{-1}$$

## Enthalpy of Formation

Krasnow<sup>1</sup> has reported calculations of the ionization potentials (IP) for the monohalides (MX, where X = F, Cl, Br, and I) of Group IIA elements (M = Mg, Ca, Sr, and Ba). Based on his data we obtain graphically the value IP(BeCl, g) = 8.9 ± 0.5 eV. The value of  $\Delta_i H^{\circ}(298.15\text{ K})$  is derived as  $21.9 \pm 15 \text{ kcal}\cdot\text{mol}^{-1}$ , using  $\Delta_i H^{\circ}$ , yielding  $\Delta_i F^{\circ}(298.15\text{ K}) = 13.9 \text{ kcal}\cdot\text{mol}^{-1}$ . Beckett<sup>2</sup> reported the ionization potential of BeCl(g) to be approximately  $9 \pm 1 \text{ eV}$ , yielding  $\Delta_i F^{\circ}(298.15\text{ K}) = 222 \pm 23 \text{ kcal}\cdot\text{mol}^{-1}$ . Hildenbrand<sup>3</sup> measured the appearance potential (AP) of BeCl<sup>+</sup>(g) to be  $9.5 \pm 0.7 \text{ kcal}\cdot\text{mol}^{-1}$  which is on the same order of the above IP values, and assumed that IP(BeCl<sup>+</sup>, g) = AP(BeCl<sup>+</sup>, g) =  $9.5 \pm 0.7 \text{ eV}$ . Using this IP value, we obtain  $\Delta_i H^{\circ}(298.15\text{ K}) = 23.4 \pm 20 \text{ kcal}\cdot\text{mol}^{-1}$  which is adopted.

## Heat Capacity and Entropy

The six electronic states are obtained from Fougert.<sup>1</sup> The electronic levels are estimated by comparison with those for BeCl(g) and LiCl(g). B<sub>e</sub> and  $\alpha_e$  are calculated using the method suggested by Herzberg.<sup>5</sup> The bond distance is estimated.\*

## References

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T/K	$C_p^*$	$S^*$	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^* = 0.1 \text{ MPa}$	
			$H^{\circ}-H^{\circ}(T_r)/T$	$-[G^{\circ}-H^{\circ}(T_r)]/T$	$H^{\circ}-H^{\circ}(T_r)$	$\Delta_i G^*$
0	0	0	INFINITE	-8.990	970.392	
100	29.155	179.796	-6.081	-3.111	945.379	-163.626
200	30.594	200.327	215.883	-1.553	945.379	-164.569
250	31.734	207.277	213.488	0	979.036	945.379
298.15	32.744	212.953	212.955	0.061	979.093	945.379
300	32.780	213.157	212.955	1.722	980.057	939.339
350	33.652	218.278	213.358	2.426	933.574	-140.204
400	34.356	222.820	215.443	5.155	981.814	-121.912
450	34.918	226.900	216.777	6.913	921.539	-107.673
500	35.370	230.603	216.777	8.442	921.531	-96.272
600	36.036	237.115	219.639	10.496	984.206	-99.161
700	36.495	242.706	222.544	14.113	985.685	-66.990
800	36.828	247.602	217.780	17.780	883.034	-57.700
900	37.082	251.955	228.093	21.476	880.700	-50.534
1000	37.287	255.873	230.678	25.195	985.754	-44.794
1100	37.463	259.425	233.133	28.933	990.827	-40.092
1200	37.628	262.702	235.463	32.687	991.916	-36.169
1300	37.800	267.721	237.676	36.459	992.934	-32.846
1400	37.993	268.529	239.780	40.248	983.879	-29.995
1500	38.224	271.158	241.785	44.059	994.752	-27.522
1600	38.503	273.633	243.699	47.894	981.021	777.197
1700	38.842	278.209	245.530	51.761	764.422	-25.373
1800	39.247	281.729	247.284	55.655	783.318	-23.488
1900	39.722	280.343	248.968	59.613	984.490	738.675
2000	40.267	282.394	250.588	63.612	985.686	725.706
2100	40.881	284.373	252.150	67.669	986.913	712.577
2200	41.558	286.290	253.659	71.790	988.369	66.610
2300	42.290	288.154	255.118	75.982	989.483	686.442
2400	43.068	290.970	256.533	80.250	990.836	673.238
2500	43.883	291.744	257.906	84.597	992.240	659.976
2600	44.722	293.482	259.241	89.027	993.656	646.657
2700	45.575	295.186	260.541	93.542	995.206	633.281
2800	46.431	296.859	261.808	98.142	705.814	626.070
2900	47.278	298.503	263.045	102.828	708.496	623.175
3000	48.108	300.120	264.254	107.597	711.248	620.186
3100	48.910	301.710	265.437	112.448	714.065	617.104
3200	49.677	303.765	266.559	117.378	716.944	613.931
3300	50.403	304.815	270.382	122.382	719.879	610.666
3400	51.082	306.330	268.843	127.457	722.866	607.312
3500	51.709	307.820	269.935	132.597	725.897	603.870
3600	52.283	309.285	271.008	137.797	730.070	596.724
3700	52.802	310.724	272.062	143.052	732.070	596.724
3800	53.264	312.139	273.058	148.352	735.550	593.024
3900	53.670	313.528	274.117	153.703	738.348	589.242
4000	54.022	314.891	275.119	159.088	741.509	585.378
4100	54.320	316.229	276.106	164.505	747.845	581.436
4200	54.568	317.541	277.077	169.950	757.416	577.416
4300	54.768	318.827	278.033	175.417	751.009	573.321
4400	54.922	320.092	278.974	180.922	754.161	569.152
5000	55.205	321.152	281.088	186.400	757.298	564.912
5100	55.016	328.222	285.189	191.467	755.550	564.912
5200	54.928	329.289	286.227	224.964	778.464	563.358
5300	55.108	322.534	280.815	210.415	760.602	562.366
5400	54.703	323.720	281.716	197.421	763.070	556.225
5500	54.572	322.561	282.603	202.936	766.569	551.782
5600	54.431	326.018	283.477	208.450	769.599	547.276
5700	54.197	333.343	288.246	213.922	772.594	542.709
5800	54.127	334.305	290.046	224.842	789.673	540.176
5900	53.968	336.172	290.817	235.693	794.991	540.185
6000	53.805	337.077	292.329	268.492	800.109	494.069

CURRENT: June 1968 (1 bar)

PREVIOUS: June 1968 (1 atm)

## Beryllium Chloride Fluoride (BeClF)

## IDEAL GAS

$$\Delta_f H^\circ(0\text{ K}) = [-574 \pm 42] \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15\text{ K}) = [246.49] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

Vibrational Frequencies and Degeneracies	
v, cm <sup>-1</sup>	C <sub>v</sub>
[500] (1)	
[270] (2)	
[130] (1)	

Ground State Quantum Weight: 1

Point Group: C<sub>∞v</sub>

Bond Distances: Be-Cl = [1.77] Å;

Be-F = [1.43] Å

Bond Angle: Cl-Be-F = [180]<sup>o</sup>Rotational Constant: B<sub>0</sub> = [0.129706] cm<sup>-1</sup>

**Enthalpy of Formation**  
The enthalpy of formation was estimated by assuming  $\Delta_f H^\circ = 0$  for the reaction  $\text{BeF}_2 + \text{BeCl}_2 \rightarrow 2\text{BeClF}$ .

## Heat Capacity and Entropy

The structure, bond lengths and frequencies were all estimated from the properties of  $\text{BeCl}_2$  and  $\text{BeF}_2$ .

T/K	C <sub>p</sub> <sup>*</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K			Standard State Pressure = p <sup>*</sup> = 0.1 MPa		
		S°	-(G° - H°(T))/T	H° - H°(T <sub>r</sub> )	Δ <sub>f</sub> G°	Δ <sub>f</sub> H°	Δ <sub>f</sub> S°
0	0	0	0	-11,704	-573,977	-573,977	INFINITE
100	34.801	200,224	286,166	-8,654	-573,876	-573,876	300,808
200	44.337	227,702	250,869	-4,633	-573,416	-578,060	150,974
250	47.364	237,561	247,289	-2,332	-573,267	-579,240	121,026
288.15	49.413	246,486	246,486	0.	-573,208	-580,397	101,683
300	49.483	246,792	246,487	0.091	-573,207	-580,442	101,064
350	51.183	254,552	247,096	2,609	-573,221	-581,647	86,806
400	52.601	261,482	248,469	5,205	-573,280	-582,847	76,112
450	53.805	257,748	250,268	7,856	-573,368	-584,038	67,793
500	54.832	273,472	252,307	10,583	-573,474	-585,218	61,137
600	56.463	283,621	260,701	16,152	-574,019	-587,544	51,150
700	57.663	292,419	261,189	21,861	-574,357	-592,060	44,013
800	58.556	300,180	265,588	27,674	-574,746	-594,250	34,489
900	59.231	307,118	269,924	33,565	-575,192	-596,394	31,132
1000	59.749	313,387	273,872	39,515	-575,348	-598,490	28,420
1100	60.152	319,101	277,777	45,511	-576,283	-600,536	26,141
1200	60,472	324,349	281,197	51,543	-576,938	-602,531	24,210
1300	60.729	329,200	284,890	57,603	-577,613	-604,473	22,553
1400	60.938	333,708	288,218	63,687	-578,491	-606,359	21,115
1500	61.109	337,919	291,392	69,789	-578,491	-607,662	19,838
1600	61.252	341,867	294,425	75,908	-593,933	-608,502	18,697
1700	61.373	345,584	297,326	82,039	-594,527	-613,422	17,682
1800	61.474	349,095	300,106	88,182	-595,142	-609,307	16,772
1900	61.562	352,421	302,778	94,334	-595,781	-610,077	15,953
2000	61.636	355,581	305,334	100,494	-596,443	-610,812	
2100	61.701	358,590	307,799	106,661	-597,128	-611,514	
2200	61.758	361,462	310,174	112,834	-597,839	-612,182	
2300	61.808	364,208	312,464	119,012	-598,566	-612,818	
2400	61.851	366,840	314,675	125,195	-599,318	-613,993	
2500	61.890	369,365	316,812	131,382	-600,050	-613,993	
2600	61.925	371,793	318,881	137,573	-600,883	-614,534	
2700	61.952	374,131	320,834	143,767	-601,696	-615,044	
2800	61.983	376,381	322,826	149,964	-603,488	-609,300	
2900	62.008	378,560	324,711	156,163	-599,155	-609,300	
3000	62.031	380,663	326,541	162,365	-603,054	-609,017	
3100	62.051	382,697	328,320	168,570	-602,839	-608,886	
3200	62.070	384,667	330,030	174,776	-602,626	-608,761	
3300	62.087	386,567	331,734	180,984	-602,413	-588,644	
3400	62.102	388,431	333,375	187,193	-602,203	-548,533	
3500	62.117	390,217	334,973	193,404	-601,995	-538,428	
3600	62.130	391,982	336,533	199,616	-601,790	-528,229	
3700	62.142	393,684	338,035	205,830	-601,583	-518,235	
3800	62.153	395,342	339,540	212,045	-601,393	-508,148	
3900	62.163	396,956	340,922	218,261	-601,203	-498,065	
4000	62.173	398,530	342,411	224,477	-601,020	-487,986	
4100	62.182	400,066	343,798	230,695	-600,845	-477,913	
4200	62.190	401,564	345,156	236,914	-600,678	-467,843	
4300	62.198	403,028	346,485	243,133	-600,522	-457,778	
5000	62.239	412,412	355,074	248,153	-600,377	-447,716	
5100	62.244	413,644	356,211	292,911	-600,136	-437,657	
5200	62.248	414,853	357,327	299,136	-600,765	-367,302	
5300	62.252	416,039	358,423	305,361	-600,750	-357,255	
5400	62.256	417,202	359,501	311,586	-600,725	-347,207	
5500	62.260	418,345	360,501	317,812	-600,700	-337,160	
5600	62.263	419,467	361,603	324,038	-600,683	-327,111	
5700	62.265	420,569	362,627	330,264	-600,661	-317,061	
5800	62.270	421,652	363,636	336,491	-600,632	-307,008	
5900	62.272	422,716	364,628	342,718	-600,615	-296,934	
6000	62.275	423,763	365,605	348,946	-600,597	-286,839	

PREVIOUS: June 1965 (1 atm)

CURRENT: June 1965 (1 bar)

## Beryllium Chloride Fluoride (BeClF)

Be<sub>2</sub>Cl<sub>1</sub>F<sub>1</sub>(g)

**Beryllium Chloride, Alpha ( $\alpha$ -BeCl<sub>2</sub>)****CRYSTAL( $\alpha$ )** **$M_r = 79.91818$  Beryllium Chloride, Alpha (BeCl<sub>2</sub>)**

$$S^\circ(298.15 \text{ K}) = 82.68 \pm 0.25 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{fs} = 688 \text{ K}$$

$$\begin{aligned} \Delta_f H^\circ(0 \text{ K}) &= -491.8 \pm 3.3 \text{ kJ}\cdot\text{mol}^{-1} \\ \Delta_f H^\circ(298.15 \text{ K}) &= -490.9 \pm 3.3 \text{ kJ}\cdot\text{mol}^{-1} \\ \Delta_{e,a} H^\circ &= 8.66 \pm 0.25 \text{ kJ}\cdot\text{mol}^{-1} \end{aligned}$$

**Enthalpy of Formation**

Johnson and Gilliland<sup>1</sup> have directly reacted beryllium and chlorine and obtained  $\Delta_f H^\circ = -118.03 \pm 0.56 \text{ kcal}\cdot\text{mol}^{-1}$  though the crystal form of the product was unknown. Gross, Heyman, Greene and Bingha<sup>2</sup> also by direct combustion of the elements obtain  $\Delta_f H^\circ = -117.1 \pm 0.4 \text{ kcal}\cdot\text{mol}^{-1}$ . The crystal form of the sample was deduced to be  $\alpha'$  by a comparison experiment, the assumption is made here that  $\alpha$  and  $\alpha'$  are identical. Thompson, Sinkle and Stull<sup>3</sup> by solution calorimetry report a  $\Delta_f H^\circ = -118.25 \pm 0.5 \text{ kcal}\cdot\text{mol}^{-1}$ . Initially this sample was reported to be of unknown crystal form. However, Sinkle<sup>4</sup> reports that an x-ray of the sample used has been reinterpreted, in the light of more recent data, as being approximately 50%  $\alpha'$  and 50%  $\beta$ . Using the enthalpies of transition adopted for these tables, enthalpies of formation of  $-117.3 \pm 0.8 \text{ kcal}\cdot\text{mol}^{-1}$  for  $\alpha$  and  $-118.6 \pm 0.8 \text{ kcal}\cdot\text{mol}^{-1}$  for  $\beta$  have been adopted as being the most consistent with all measurements.

**Heat Capacity and Entropy**

McDonald and Oetting<sup>5</sup> have measured the heat capacity of the  $\alpha'$  form from 13 and 304 K and the enthalpy (relative to the  $\alpha'$  form) from 676 to 688 K. The assumption has been made that the  $\alpha$  and  $\alpha'$  forms are identical and the heat capacity curve between 304 and 676 K has been estimated graphically. The entropy was obtained by integration of the heat capacity curve assuming  $S^\circ(T|3 \text{ K}) = 0.16 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . The sample was identified as  $\alpha'$  by x-ray diffraction both before and after the experiments.

**Fusion Data**

The temperature and enthalpy of melting were reported by McDonald and Oetting.<sup>5</sup> Several investigations of the melting point are in disagreement mainly due to the uncertainty of the crystal form of the material and a solid state transition just below the pure  $\alpha$ -liquid melting point.

**Sublimation Data**

The adopted enthalpy of sublimation was calculated from that of the  $\beta$  form and enthalpy of the  $\alpha$ - $\beta$  transition at 298.15 K.

**References**

- <sup>1</sup>W. H. Johnson and A. A. Gilliland, J. Res. Natl. Bur. Stand., **65A**, 59 (1961).
- <sup>2</sup>P. Gross, C. Heyman, P. D. Greene and J. T. Bingham, Fulmer Research Institute, Report R. 163/SR.1/Sept. 1964 under Contract AF61 (052)-447.
- <sup>3</sup>C. J. Thompson, G. C. Sinkle and D. R. Stull, J. Chem. Eng. Data **7**, 380 (1962).
- <sup>4</sup>G. C. Sinkle, personal communication, (February 1965).
- <sup>5</sup>R. A. McDonald and F. L. Oetting, J. Phys. Chem., **69**, 3839 (1965).

**Be<sub>2</sub>Cl<sub>2</sub>(cr)**

		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$				Standard State Pressure = $p^* = 0.1 \text{ MPa}$			
		$\frac{\partial H}{\partial T} = \frac{1}{2} K^\circ \text{ mol}^{-1}$		$S^\circ - [C^\circ - H(T)]/T$		$H^\circ - H(T)/T$		$\Delta_f H^\circ$	
		$T \text{ K}$	$C^\circ$					$\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_f C^\circ$
		0	0	0	0	0	0	-491.795	-491.795
		100	33.660	28.974	131.942	-10.297	-491.795	-491.054	-249.165
		200	53.555	59.036	88.261	-5.845	-492.228	-461.011	-120.455
		298.15	64.852	82.676	82.676	0.	-490.930	-446.254	78.182
		300	65.019	83.078	82.677	0.120	-445.977	-77.651	
		400	72.760	102.907	85.329	7.031	-489.303	-431.234	56.313
		500	77.530	119.678	90.566	14.536	-487.433	-416.927	43.536
		600	80.082	134.040	96.544	22.437	-485.471	-403.007	35.085
		688.000	81.278	145.083	102.148	29.539	---	ALPHA	LIQUID
		700	81.358	146.489	102.986	30.515	-483.457	-389.422	29.059
		800	82.257	157.413	109.042	38.697	-476.125	-24.538	
		900	83.023	167.146	114.967	46.961	-471.471	-363.074	
		1000	83.680	175.929	120.631	55.297	-477.603	-350.239	21.072
		1100	84.230	183.931	126.027	63.694	-475.728	-337.593	18.295
		1200	84.672	191.280	131.163	72.140	-473.902	-323.117	16.031
		1300	85.007	198.071	136.052	80.625	-472.134	-312.790	14.152
		1400	85.234	204.380	140.710	89.138	-470.435	-300.597	12.568
		1500	85.354	210.265	145.153	97.658	-468.817	-288.523	11.215

$$T_{fs} = 688 \text{ K}$$

PREVIOUS:

CURRENT: June 1965

**Beryllium Chloride, Alpha (BeCl<sub>2</sub>)**

**Beryllium Chloride, Beta ( $\beta$ -BeCl<sub>2</sub>)****CRYSTAL( $\beta$ )**

$$\begin{aligned} S^\circ(298.15 \text{ K}) &= 75.81 \pm 0.21 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1} \\ T_{\text{fs}} &= [682] \text{ K} \\ T_{\text{ts}} &= 676 \text{ K } (\beta \rightarrow \alpha) \end{aligned}$$

**Enthalpy of Formation**See the  $\alpha$ -crystal table for details.**Heat Capacity and Entropy**

McDonald and Oetting<sup>1</sup> have measured the heat capacity of the  $\beta$ -form from 298 to 676 K. The entropy was obtained by integration of the heat capacity curve based on  $S^\circ(13 \text{ K}) = 0.06 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . The sample was identified as  $\beta$ -BeCl<sub>2</sub> both before and after the low temperature experiments.

**Fusion Data**

The temperature and enthalpy of melting were obtained from cross over point of the tables for  $\beta$ -BeCl<sub>2</sub> and liquid BeCl<sub>2</sub>.

**Transition Data**

The temperature of the  $\beta \rightarrow \alpha$  transition was obtained from McDonald and Oetting.<sup>1</sup> The enthalpy of the transition is a function of the heat capacity curve chosen for  $\alpha$ -BeCl<sub>2</sub> between 298 and 676 K. A straight line interpolation was used by McDonald and Oetting, which gives a different result (1.49 kcal/mol<sup>-1</sup>) than the curve employed here. It should also be noted that the transitional enthalpy is not included in this table, which is for  $\beta$ -BeCl<sub>2</sub> only.

**Sublimation Data**

The enthalpy of sublimation was determined by 2nd and 3rd law analysis of vapor pressure data as described fully on the table for BeCl<sub>2</sub>(g).

**References**

- <sup>1</sup>R. A. McDonald and F. L. Oetting, J. Phys. Chem., 69, 3839 (1965).

		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$			Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$		
		$\Delta_f H^\circ(0 \text{ K}) = -496.5 \pm 3.3 \text{ kJ}\cdot\text{mol}^{-1}$		$\Delta_f H^\circ(298.15 \text{ K}) = -496.2 \pm 3.3 \text{ kJ}\cdot\text{mol}^{-1}$		$\Delta_f H^\circ = [15.27 \pm 0.63] \text{ kJ}\cdot\text{mol}^{-1}$	
		$\Delta_f H^\circ = [6.82 \pm 0.63] \text{ kJ}\cdot\text{mol}^{-1}$		$S^\circ = [G^\circ - H^\circ(T)]/T$		$H^\circ - H^\circ(T)$	
		$T/K$	$C_p^\circ$	$J\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$K\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_f H^\circ$
0	0	0	0	0	INFINITE	-11.418	-496.527
100	31.777	24.104	127.616	-10.351	-498.412	251.704	INFINITE
200	51.798	32.928	81.211	-5.657	-497.332	121.469	121.469
298.15	62.425	75.814	75.814	0	-496.222	78.751	78.751
300	62.593	76.201	75.815	0.116	-496.200	-449.211	78.215
400	68.701	95.099	78.350	6.700	-494.928	-433.736	56.640
500	72.802	110.900	83.374	13.788	-493.514	-418.599	43.731
600	75.814	124.449	89.075	21.224	-491.977	-403.758	35.150
700	78.157	136.327	94.995	28.933	-490.331	-389.184	29.041
800	79.936	146.385	100.833	36.841	-488.619	-374.451	24.475
900	81.379	156.387	106.487	44.910	-486.863	-360.735	20.936
1000	82.550	165.025	111.915	53.109	-485.084	-346.816	18.116
1100	83.387	172.934	117.108	61.408	-483.306	-333.075	15.816
1200	84.015	180.217	122.088	69.780	-481.555	-319.495	13.907
1300	84.475	186.961	126.803	78.205	-479.846	-306.060	12.298
1400	84.782	193.234	131.327	86.669	-478.196	-292.754	10.923
1500	84.935	199.089	135.652	93.157	-476.621	-279.564	9.735

**Beryllium Chloride ( $\text{BeCl}_2$ )****Liquid** **$\text{Be}_1\text{Cl}_2(\text{l})$** 

$$\Delta_f H^\circ(298.15 \text{ K}) = [79.727] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

 $T_{\text{m}} = 638 \text{ K}$ 

$\Delta_{\text{m}} H^\circ = 8.66 \pm 0.25 \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**

The enthalpy of formation is calculated from that of the  $\alpha$ - $\text{BeCl}_2$  by adding  $\Delta_{\text{m}} H^\circ$  and the difference in enthalpy,  $H^\circ(683 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and liquid.

**Heat Capacity and Entropy**

McDonald and Oetting have measured the enthalpy of the liquid, relative to  $\alpha$ - $\text{BeCl}_2$ , from 688 to 713 K. The heat capacity was assumed constant above this point and also below the melting point to 460 K where a glass transition was assumed. Below 416 K the heat capacity was assumed to be that of  $\beta$ - $\text{BeCl}_2$ . The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

**Fusion**

Refer to the  $\alpha$ -crystal table for details.

**Vaporization Data**

The boiling point and enthalpy of vaporization are calculated from the cross over point of the  $\text{BeCl}_2$  (l) and (g) tables. The analysis of the liquid vapor pressure data is given on the table for  $\text{BeCl}_2(\text{g})$ .

**References**

R. A. McDonald and F. L. Oetting, *J. Phys. Chem.*, **69**, 3839 (1965).

 **$M_r = 79.91818$  Beryllium Chloride ( $\text{BeCl}_2$ )**

$T/K$	$\text{Enthalpy Reference Temperature} = T_r = 298.15 \text{ K}$		$\text{Standard State Pressure} = p^* = 0.1 \text{ MPa}$	
	$C_p^\circ$	$S^\circ$	$H^\circ - H^\circ(T_r)/T$	$\Delta_f G^\circ$
298.15	62.425	79.727	79.727	0
300	62.593	80.114	79.728	0.116
400	68.701	99.012	82.263	6.700
450.100	71.356	108.819	85.103	10.912
460.100	121.420	108.819	85.103	10.912
500	121.420	118.917	87.404	15.757
600	121.420	141.054	94.557	27.898
688.000	121.420	157.671	101.591	38.583
700	121.420	159.771	102.576	40.040
800	121.420	175.984	110.756	52.182
900	121.420	190.286	118.814	64.324
1000	121.420	203.078	126.612	76.456
1100	121.420	214.651	134.098	88.608
1200	121.420	225.216	141.257	100.750
1300	121.420	234.935	148.094	112.892
1400	121.420	243.933	154.623	125.034
1500	121.420	252.310	160.859	137.176
1600	121.420	260.146	166.822	149.318
1700	121.420	267.507	172.531	161.460
1800	121.420	274.447	178.002	173.602
1900	121.420	281.012	183.252	185.744
2000	121.420	287.240	188.297	197.886

 $\log K_r$ 

$T/K$	$\text{Enthalpy Reference Temperature} = T_r = 298.15 \text{ K}$		$\text{Standard State Pressure} = p^* = 0.1 \text{ MPa}$	
	$C_p^\circ$	$S^\circ$	$H^\circ - H^\circ(T_r)/T$	$\Delta_f G^\circ$
298.15	62.425	79.727	79.727	0
300	62.593	80.114	79.728	0.116
400	68.701	99.012	82.263	6.700
450.100	71.356	108.819	85.103	10.912
460.100	121.420	108.819	85.103	10.912
500	121.420	118.917	87.404	15.757
600	121.420	141.054	94.557	27.898
688.000	121.420	157.671	101.591	38.583
700	121.420	159.771	102.576	40.040
800	121.420	175.984	110.756	52.182
900	121.420	190.286	118.814	64.324
1000	121.420	203.078	126.612	76.456
1100	121.420	214.651	134.098	88.608
1200	121.420	225.216	141.257	100.750
1300	121.420	234.935	148.094	112.892
1400	121.420	243.933	154.623	125.034
1500	121.420	252.310	160.859	137.176
1600	121.420	260.146	166.822	149.318
1700	121.420	267.507	172.531	161.460
1800	121.420	274.447	178.002	173.602
1900	121.420	281.012	183.252	185.744
2000	121.420	287.240	188.297	197.886

 $\log K_r$ 

**Beryllium Chloride ( $\text{BeCl}_2$ )**  
PREVIOUS September 1961 CURRENT June 1965

CRYSTAL( $\beta$ - $\alpha$ )-LIQUID

## Beryllium Chloride ( $\text{BeCl}_2$ )

0	to	676 K	crystal, beta
676	to	688	crystal, alpha
above		688	liquid

Refer to the individual tables for details.

$$M_r = 79.91818 \text{ Beryllium Chloride (BeCl}_2\text{)}$$

Enthalpy Reference Temperature = $T = 298.15\text{ K}$	Standard State Pressure = $p^* = 0.1\text{ MPa}$					
	$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$			$\text{kJ}\cdot\text{mol}^{-1}$		
	$C_p^*$	$S^*$	$-[G^*-H^*(T)]/T$	$H^*-H^*(T)/T$	$\Delta_i H^*$	$\Delta_i G^*$
$T/\text{K}$						
0	0.0	0.0	INFINITE	-11.979	-491.795	INFINITE
100	33.660	28.974	131.942	-10.297	-491.054	-491.795
200	53.555	59.036	88.261	-5.845	-492.228	-477.011
298.15	64.852	82.676	82.676	0.	-490.903	-446.254
300	65.019	83.078	82.677	0.120	-490.903	-445.977
400	72.760	102.907	83.259	7.031	-489.720	-431.234
500	77.530	119.678	90.556	14.556	-487.453	-416.927
600	80.082	134.040	96.644	22.437	-485.471	-403.007
688.000	81.278	145.083	102.148	29.539	-	-
688.000	121.420	157.671	102.148	38.200	-	-
700	121.420	159.771	103.118	39.657	-474.314	-389.578
800	121.420	175.984	111.235	51.799	-463.500	-377.880
900	121.420	190.240	119.240	63.941	-467.540	-366.920
1000	121.420	203.078	126.995	76.083	-455.817	-356.603
1100	121.420	214.651	134.446	88.225	-454.675	-346.834
1200	121.420	225.216	141.577	100.367	-453.675	-337.613
1300	121.420	234.935	148.389	112.509	-440.250	-328.829
1400	121.420	243.935	154.896	124.651	-343.929	-310.458
1500	121.420	252.310	161.115	136.793	-342.620	-304.465
1600	121.420	260.146	167.062	148.335	-340.692	-312.465
1700	121.420	267.507	172.756	161.077	-340.095	-304.293
1800	121.420	274.447	178.215	171.219	-431.660	-296.034
1900	121.420	281.012	183.454	185.361	-422.255	-288.095
2000	121.420	287.240	188.489	197.503	-280.453	-273.097

PREFACE.

CURRENT Literature

Berillium Chloride (BeCl<sub>2</sub>)

BSCI (or II)

Beryllium Chloride (BeCl<sub>2</sub>)

## IDEAL GAS

$$\Delta H^\circ(0\text{ K}) = -361.5 \pm 10.5 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(298.15\text{ K}) = [232 \pm 4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

Source	T/K	$\Delta_{\text{exp}}H^\circ(298.15\text{ K}), \text{ kJ}\cdot\text{mol}^{-1}$	Drift $\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
1	680-740*	$33.5 \pm 0.6$	$-3.4 \pm 0.7$
2	680-740	$34.3$	$-4.7$
1	613-663	$31.6 \pm 1.6$	$-1.3 \pm 2.6$
2	638-668	$31.07$	$-7.0$
3	441-518	$31.4 \pm 0.8$	$2.5 \pm 1.7$
3	510-600*	$31.8 \pm 0.3$	$0.40 \pm 0.5$
4	460-504*	$32.45 \pm 0.4$	$0.14 \pm 0.8$

\*Points rejected due to failure of a statistical test.

## Enthalpy of Formation

The vapor pressure data over the crystal was assumed to be for the  $\beta$ -form. The 2nd and 3rd law analyses of the data are summarized below after conversion to a common process. The data were also analyzed using gaseous Gibbs energy functions based on a bending frequency of  $170 \text{ cm}^{-1}$  but no significant improvement of the results was noted.

Source	T/K	$\Delta_{\text{exp}}H^\circ(298.15\text{ K}), \text{ kJ}\cdot\text{mol}^{-1}$	2nd law	3rd law	Drift $\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
1	680-740*	$33.5 \pm 0.6$	$31.38$	$-3.4 \pm 0.7$	
2	680-740	$34.3$	$31.22$	$-4.7$	
1	613-663	$31.6 \pm 1.6$	$30.91$	$-1.3 \pm 2.6$	
2	638-668	$31.07$	$31.07$	$-7.0$	
3	441-518	$31.4 \pm 0.8$	$32.45$	$2.5 \pm 1.7$	
3	510-600*	$31.8 \pm 0.3$	$32.07$	$0.40 \pm 0.5$	
4	460-504*	$32.45 \pm 0.4$	$32.48$	$0.14 \pm 0.8$	

\*Points rejected due to failure of a statistical test.

It is obvious that there is no real agreement between the data sets, and some of this is undoubtedly due to the difficulty of keeping a single crystal form throughout a series of measurements. It is also doubtful that water vapor was adequately excluded in some experiments. We have adopted the only piece of work which shows adequate 2nd and 3rd law agreement, and no 3rd law trend, that is  $\Delta_{\text{exp}}H^\circ = 32.5 \pm 1 \text{ kcal}\cdot\text{mol}^{-1}$  from. It is interesting to note that all the other data can be made much more precise and its drift removed if a constant pressure is added to all points. The addition which varied from 20-30% of the lowest pressure in each data set serves to indicate the magnitude of possible systematic errors.

## Heat Capacity and Entropy

The linear structure of BeCl<sub>2</sub>(g) has been confirmed by the electric deflection experiments of Buchler.<sup>5</sup> The bond length was obtained from the electron diffraction data of Akishin, Spiridonov and Sobelev.<sup>6</sup> Buchler and Klemperer<sup>7</sup> have reported the infra-red spectrum and assigned 1113 as the asymmetric stretch  $v_3$  and 482 as the bending frequency  $v_2$ . However, Nelson<sup>8</sup> using matrix isolation experiments, has shown this second band to be due to beryllium chloride solid. The unobserved frequencies were estimated from a valence force field treatment assuming that the ratio of stretching to bending force constant was 50:1, the same as for BeF<sub>2</sub>(g). This gives 230 cm<sup>-1</sup> for  $v_2$  and 375 cm<sup>-1</sup> for the symmetric stretch.

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M<sub>r</sub> = 79.91818 Beryllium Chloride (BeCl<sub>2</sub>)

Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^* = 0.1 \text{ MPa}$	
$C_p^*$	$S^*$	$-[G^* - H^*(T)]/T$	$H^* - H^*(T_r)/T_r$
0	0	INFINITE	-12.322
100	37.378	202.989	-9.183
200	47.677	232.467	-4.873
250	49.785	243.300	-2.443
298.15	51.622	252.232	0.
300	51.685	252.572	0.096
350	53.221	260.638	2.719
400	54.497	267.831	5.413
450	55.563	274.313	8.166
500	56.455	280.215	10.967
600	57.830	290.636	16.682
700	58.809	299.629	22.510
800	59.517	307.530	28.438
900	60.042	314.572	34.417
1000	60.438	320.920	40.442
1100	60.744	326.695	46.421
1200	60.983	331.991	52.588
1300	61.174	336.880	58.697
1400	61.229	341.419	64.822
1500	61.453	345.653	70.961
1600	61.560	349.625	76.112
1700	61.548	353.346	81.723
1800	61.722	356.885	87.196
1900	61.785	360.224	93.567
2000	61.840	363.395	99.500
2100	61.887	366.413	104.992
2200	61.928	369.293	111.955
2300	61.964	372.047	119.715
2400	61.995	374.683	126.568
2500	62.023	377.216	132.769
2600	62.048	379.649	138.972
2700	62.070	381.991	145.221
2800	62.090	384.249	150.182
2900	62.108	386.428	153.084
3000	62.124	388.534	163.808
3100	62.139	390.571	170.021
3200	62.154	392.544	176.236
3300	62.164	394.457	182.451
3400	62.176	396.313	188.668
3500	62.186	398.115	194.887
3600	62.195	399.867	204.005
3700	62.204	401.571	207.537
3800	62.212	403.230	213.546
3900	62.219	404.846	219.768
4000	62.226	406.422	249.924
4100	62.232	407.938	351.321
4300	62.244	410.458	352.687
4400	62.249	411.354	340.025
4500	62.253	413.753	356.617
4600	62.258	415.121	357.874
4700	62.262	416.460	359.106
4800	62.266	417.771	360.315
4900	62.270	419.055	361.501
5000	62.273	420.313	362.664
5100	62.277	421.546	363.807
5200	62.280	422.755	364.929
5300	62.283	423.942	366.031
5400	62.285	425.106	367.114
5500	62.288	426.249	368.179
5600	62.290	427.371	369.226
5700	62.293	428.474	370.256
5800	62.295	429.557	371.269
5900	62.297	430.622	372.266
6000	62.299	431.669	373.247

Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^* = 0.1 \text{ MPa}$	
$C_p^*$	$S^*$	$-[G^* - H^*(T)]/T$	$H^* - H^*(T_r)/T_r$
0	0	INFINITE	-361.451
100	37.378	202.989	-9.183
200	47.677	232.467	-4.873
250	49.785	243.300	-2.443
298.15	51.622	252.232	0.
300	51.685	252.572	0.096
350	53.221	260.638	2.719
400	54.497	267.831	5.413
450	55.563	274.313	8.166
500	56.455	280.215	10.967
600	57.830	290.636	16.682
700	58.809	299.629	22.510
800	59.517	307.530	28.438
900	60.042	314.572	34.417
1000	60.438	320.920	40.442
1100	60.744	326.695	46.421
1200	60.983	331.991	52.588
1300	61.174	336.880	58.697
1400	61.229	341.419	64.822
1500	61.453	345.653	70.961
1600	61.560	349.625	76.112
1700	61.548	353.346	81.723
1800	61.722	356.885	87.196
1900	61.785	360.224	93.567
2000	61.840	363.395	99.500
2100	61.887	366.413	104.992
2200	61.928	369.293	111.955
2300	61.964	372.047	119.715
2400	61.995	374.683	126.568
2500	62.023	377.216	132.769
2600	62.048	379.649	138.972
2700	62.070	381.991	145.221
2800	62.090	384.249	150.182
2900	62.108	386.428	153.084
3000	62.124	388.534	163.808
3100	62.139	390.571	170.021
3200	62.154	392.544	176.236
3300	62.164	394.457	182.451
3400	62.176	396.313	188.668
3500	62.186	398.115	194.887
3600	62.195	399.867	204.005
3700	62.204	401.571	207.537
3800	62.212	403.230	213.546
3900	62.219	404.846	219.768
4000	62.226	406.422	249.924
4100	62.232	407.938	351.321
4300	62.244	410.458	352.687
4400	62.249	411.354	344.025
4500	62.253	413.753	356.617
4600	62.258	415.121	357.874
4700	62.262	416.460	359.106
4800	62.266	417.771	360.315
4900	62.270	419.055	361.501
5000	62.273	420.313	362.664
5100	62.277	421.546	363.807
5200	62.280	422.755	364.929
5300	62.283	423.942	366.031
5400	62.285	425.106	367.114
5500	62.288	426.249	368.179
5600	62.290	427.371	369.226
5700	62.293	428.474	370.256
5800	62.295	429.557	371.269
5900	62.297	430.622	372.266
6000	62.299	431.669	373.247

CURRENT June 1965 (1 atm)

Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^* = 0.1 \text{ MPa}$	
$C_p^*$	$S^*$	$-[G^* - H^*(T)]/T$	$H^* - H^*(T_r)/T_r$
0	0	INFINITE	-361.451
100	37.378	202.989	-9.183
200	47.677	232.467	-4.873
250	49.785	243.300	-2.443
298.15	51.622	252.232	0.
300	51.685	252.572	0.096
350	53.221	260.638	2.719
400	54.497	267.831	5.413
450	55.563	274.313	8.166
500	56.455	280.215	10.967
600	57.830	290.636	16.682
700	58.809	299.629	22.510
800	59.517	307.530	28.438
900	60.042	314.572	34.417
100			

Ground State Configuration:  $2s^2$   
 $S^o(298.15 \text{ K}) = [205.75 \pm 0.04] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

$$\Delta H^o(0 \text{ K}) = -172.2 \pm 8 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^o(298.15 \text{ K}) = -169.9 \pm 8 \text{ kJ}\cdot\text{mol}^{-1}$$

Electronic Levels and Quantum Weights		
$\epsilon_r$ , cm <sup>-1</sup>	$\epsilon$ , cm <sup>-1</sup>	$\sigma$ , 1
0	2	50419
33180	4	63916
49573	2	66573
		[4]

$$\omega_e = 1265.9 \text{ cm}^{-1}$$

$$B_e = 1.489 \text{ cm}^{-1}$$

$$\alpha_e = 0.0176 \text{ cm}^{-1}$$

#### Enthalpy of Formation

$\Delta_e H^o$  is based on 3rd law analysis of  $K_p$  data for three gas-phase reactions observed mass spectrometrically by Hildenbrand *et al.*<sup>1,2</sup> Our analysis is summarized below. Also included are data for heterogeneous reaction of Be(cr) with BeF<sub>4</sub>(g), observed with a molecular-flow-effusion method by Greenbaum *et al.*<sup>3</sup> The mutual consistency of the gas-phase results prompts us to adopt a weighted average of  $-40.6 \pm 2$  kcal·mol<sup>-1</sup> rather than the mean value of  $-53.1$  kcal·mol<sup>-1</sup> derived from the heterogeneous reaction.

Analogous studies of BeCl(g) gave a similar discrepancy which was reaffirmed by new transport studies of Gross and Lewin.<sup>4</sup> These authors suggested that transport via (Becl)<sub>2</sub> provides a possible, but inconclusive, explanation of the discrepancy. This explanation may also apply to BeF, but new data would be needed to establish this.

The adopted  $\Delta_e H^o$  yields  $D_0^o = 5.98 \pm 0.1$  eV which is consistent with spectroscopic results within their probable uncertainties.<sup>5</sup> Spectroscopic values<sup>1,5</sup> include 6.3 or  $6.0 \pm 0.5$  eV (from A<sup>2</sup>T) and 5.3 cal·K<sup>-1</sup>·mol<sup>-1</sup> (from X<sup>2</sup>Σ). Rationales have been given<sup>4-6</sup> for the lowness of the value derived from the ground state. Recent calculations<sup>7,8</sup> showed that the ground-state potential energy curve is consistent with  $D_0^o = 5.85$  eV. The flow-effusion data<sup>9</sup> yield 6.52 cal·K<sup>-1</sup>·mol<sup>-1</sup>.

$$\Delta H^o(298.15 \text{ K}), \text{ kcal}\cdot\text{mol}^{-1}$$

$$\Delta H^o(298.15 \text{ K}), \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\frac{\partial \Delta H^o}{\partial T}(298.15 \text{ K}), \text{ kcal}\cdot\text{mol}^{-1}$$

$$\frac{\partial \Delta H^o}{\partial T}(298.15 \text{ K}), \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\frac{\partial \Delta H^o}{\partial S}(298.15 \text{ K}), \text{ kcal}\cdot\text{mol}^{-1}$$

$$\frac{\partial \Delta H^o}{\partial S}(298.15 \text{ K}), \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\frac{\partial \Delta H^o}{\partial V}(298.15 \text{ K}), \text{ kcal}\cdot\text{mol}^{-1}$$

$$\frac{\partial \Delta H^o}{\partial V}(298.15 \text{ K}), \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

Source	Method	Reaction*	T/K	2nd law	3rd law	cal·K <sup>-1</sup> ·mol <sup>-1</sup>	cal·K <sup>-1</sup> ·mol <sup>-1</sup>	ΔH <sup>o</sup> (298.15 K), kcal·mol <sup>-1</sup>	ΔH <sup>o</sup> (298.15 K), cal·K <sup>-1</sup> ·mol <sup>-1</sup>
Hildenbrand <sup>1</sup>	Mass Spec.	A	1438-1609	25.9 ± 9	28.28 ± 2	-1.6 ± 5.7	-41.86 ± 1.3	29.09 ± 2	1.5 ± 1.5
		A	1321-1518	31.2 ± 2	30.4 ± 3	24.	-41.46 ± 1.3	-7.86 ± 2.1	-40.8 ± 1.7
		A	1427-1443	-4.1	-4.1	-37.46 ± 3.0	-0.8 ± 2.1	-8.7 ± 3	-38.3 ± 3.8
		B	1321-1503	-6.7 ± 3	-7.86 ± 2	20.	-38.3 ± 3.8	-8.2 ± 3	-38.9 ± 3.4
		B	1423-1443	-3.8	-3.8	8.	-38.9 ± 3.4	-8.2 ± 3	-39.5 ± 3.4
		C	1423-1443	12.7	12.7	8.47 ± 3	-52.8 ± 1.6	-52.8 ± 1.6	-52.8 ± 1.6
		D	1420-1525	97. ± 10	80.7 ± 3	-1.2 ± 3.7	-53.4 ± 1.6	-83. ± 6	-83. ± 6
		E	1570-1675						



#### Heat Capacity and Entropy

Rotational constants are from a new analysis of the A-X system by Walker and Barrow.<sup>9</sup> Vibrational constants are those derived by Novikov and Gurvich<sup>10</sup> and Gurvich<sup>11</sup> from data of Tseytlin et al.<sup>12</sup> Excited states are from Novikov and Gurvich.<sup>10</sup> We assume that the two highest states are 2Π as postulated by Walker and Barrow<sup>9</sup> from comparison with quantum calculations.<sup>12</sup>

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<sup>10</sup>M. M. Novikov and L. V. Gurvich, Opt. Spectrosc. **5**, 521 (1958).

<sup>11</sup>V. M. Tseytlin, L. N. Tunitskii and M. M. Novikov, *Opt. Spektrosk.* **23**, 323 (1967).

<sup>12</sup>T. E. Walker and W. G. Richards, *Proc. Phys. Soc.* **92**, 285 (1967).

Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K										Standard State Pressure = p <sup>o</sup> = 0.1 MPa		
T/K	$C_p^o$	$S^o$	$-[G^o - H^o(T, J)]/T$	$H^o - H^o(T_r)$			$k\cdot\text{mol}^{-1}$			$\Delta_e G^o$	$\log K_r$	
				$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$			
0	0	0	0	0	0	0	0	0	0	-8.711	-172.237	
100	29.109	173.800	173.865	-5.807	-170.825	-170.856	-170.833	-170.821	-170.817	-170.827	-93.832	
200	29.204	193.980	208.457	-2.893	-169.954	-168.852	-169.831	-169.816	-169.800	-169.824	-40.449	
250	29.454	205.530	206.241	-1.428	-169.387	-169.170	-169.387	-169.374	-169.361	-169.387	-19.170	
298.15	29.872	205.751	205.751	0	-169.387	-169.387	-169.387	-169.387	-169.387	-169.387	-34.535	
300	29.891	205.536	205.752	0.055	-169.387	-169.387	-169.387	-169.387	-169.387	-169.387	-10.583	
350	30.461	210.086	206.118	1.564	-170.039	-170.039	-170.039	-170.039	-170.039	-170.039	-30.508	
400	31.091	214.694	206.538	3.102	-170.279	-170.134	-170.279	-170.279	-170.279	-170.279	-27.134	
450	31.725	218.393	208.009	4.673	-170.569	-170.454	-170.569	-170.569	-170.569	-170.569	-24.661	
500	32.327	221.767	209.218	6.274	-170.853	-170.971	-170.853	-170.853	-170.853	-170.853	-22.679	
600	33.379	227.757	211.821	9.561	-171.609	-172.265	-171.609	-171.609	-171.609	-171.609	-19.698	
700	34.217	232.968	212.083	12.943	-174.341	-173.241	-174.341	-174.341	-174.341	-174.341	-15.948	
900	35.387	241.720	219.595	19.913	-174.446	-173.056	-174.446	-174.446	-174.446	-174.446	-14.688	
1000	35.795	245.470	221.998	23.472	-175.115	-174.783	-175.115	-175.115	-175.115	-175.115	-13.674	
1100	36.124	248.898	224.289	26.169	-176.149	-175.401	-176.149	-176.149	-176.149	-176.149	-12.840	
1200	36.393	252.053	226.473	30.695	-177.254	-176.721	-177.254	-177.254	-177.254	-177.254	-12.141	
1300	36.617	254.975	228.555	34.346	-178.433	-178.433	-178.433	-178.433	-178.433	-178.433	-11.032	
1400	36.806	257.696	230.540	38.018	-179.689	-179.689	-179.689	-179.689	-179.689	-179.689	-10.583	
1500	36.968	260.241	232.436	41.707	-181.026	-181.026	-181.026	-181.026	-181.026	-181.026	-10.583	
1600	37.109	262.631	234.250	45.411	-186.982	-186.982	-186.982	-186.982	-186.982	-186.982	-10.171	
1700	37.233	264.885	235.986	49.126	-188.663	-188.663	-188.663	-188.663	-188.663	-188.663	-9.791	
1800	37.343	267.016	237.651	52.837	-190.206	-190.206	-190.206	-190.206	-190.206	-190.206	-9.452	
1900	37.442	269.038	239.560	56.596	-190.344	-190.344	-190.344	-190.344	-190.344	-190.344	-9.147	
2000	37.532	270.961	240.788	60.345	-190.498	-190.498	-190.498	-190.498	-190.498	-190.498	-8.871	
2100	37.615	272.794	242.679	64.102	-190.668	-190.668	-190.668	-190.668	-190.668	-190.668	-8.620	
2200	37.691	274.545	243.697	67.868	-193.353	-193.353	-193.353	-193.353	-193.353	-193.353	-8.390	
2300	37.762	276.222	245.075	71.640	-195.052	-195.052	-195.052	-195.052	-195.052	-195.052	-8.195	
2400	37.824	277.831	246.406	75.460	-196.847	-196.847	-196.847	-196.847	-196.847	-196.847	-7.804	
2500	37.901	278.564	248.942	82.928	-199.929	-199.929	-199.929	-199.929	-199.929	-199.929	-7.513	
2700	38.008	282.297	250.151	90.600	-202.516	-202.516	-202.516	-202.516	-202.516	-202.516	-6.896	
2800	38.063	283.917	252.562	94.409	-204.241	-204.241	-204.241	-204.241	-204.241	-204.241	-6.595	
3000	38.166	286.310	253.569	98.223	-207.484	-207.484	-207.484	-207.484	-207.484	-207.484	-6.295	
3100	38.215	287.562	254.645	102.678	-207.678	-207.678	-207.678	-207.678	-207.678	-207.678	-6.048	
3200	38.263	288.776	255.693	105.846	-208.828	-208.828	-208.828	-208.828	-208.828	-208.828	-5.799	
3300	38.310	289.955	256.714	109.694	-209.988	-209.988	-209.988	-209.988	-209.988	-209.988	-5.565	
3400	38.356	291.099	257.708	113.528	-210.722	-210.722	-210.722	-210.722	-210.722	-210.722	-5.344	
3600	38.446	293.394	259.625	121.208	-212.028	-212.028	-212.028	-212.028	-212.028	-212.028	-5.135	
3700	38.491	294.348	260.549	126.549	-214.870	-214.870	-214.870	-214.870	-214.870	-214.870	-4.891	
3800	38.535	295.372	261.452	126.474	-216.474	-216.474	-216.474	-216.474	-216.474	-216.474	-4.604	
3900	38.579	296.377	262.382	128.906	-218.556	-218.556	-218.556	-218.556	-218.556	-218.556	-4.384	
4000	38.623	297.354	263.198	132.762	-220.722	-220.722	-220.					

Beryllium Fluoride (BeF <sub>2</sub> )		CRYSTAL (I-I)		M <sub>r</sub> = 47.0008986 Beryllium Fluoride (BeF <sub>2</sub> )	
$\Delta_f H^\circ(0\text{ K}) = -1024.5 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$	$\Delta_f H^\circ(298.15\text{ K}) = -1026.8 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$	$T_{\text{in}} = 500\text{ K}$ (low quartz $\rightarrow$ high quartz)	$T_{\text{in}} = 825\text{ K}$	$\Delta_{\text{in}}H^\circ = 0.2201 \text{ kJ}\cdot\text{mol}^{-1}$	$\Delta_{\text{in}}H^\circ = 4.757 \text{ kJ}\cdot\text{mol}^{-1}$
<b>Enthalpy of Formation</b>					
$\Delta_f H^\circ$ is the value selected by Parker, <sup>1</sup> based on a thorough review of data for BeF <sub>2</sub> (cr, vitreous, aq) and BeO(cr). Parker's analysis remains essentially unchanged for BeO(cr) and BeF <sub>2</sub> (cr), even though the results for BeF <sub>2</sub> (HF, aq) become more negative by 0.93 kcal·mol <sup>-1</sup> due to JANAF selections for HF(aq). Three values derived for BeF <sub>2</sub> (cr) from pBeF <sub>2</sub> (cr) are changed due to JANAF auxiliary data; these values become $-246.9$ , $-246.0$ and $-247.2$ for the three paths used by Parker.					
The adopted $\Delta_f H^\circ$ was derived by combination of calorimetric data for Be(cr) + F(g) $\rightarrow$ BeF <sub>2</sub> (vitreous) and BeF <sub>2</sub> (cr) $\rightarrow$ BeF <sub>2</sub> (cr).					
Churney and Armstrong <sup>2</sup> obtained $\Delta_f H^\circ(298.15\text{ K}) = -244.32 \pm 0.8 \text{ kcal}\cdot\text{mol}^{-1}$ for vitreous BeF <sub>2</sub> by combustion in fluorine of polytetrafluoroethylene and mixtures of Be(cr) with polytetrafluoroethylene. $\Delta_f H^\circ(298.15\text{ K}, \text{cr} \rightarrow \text{vitreous}) = 1.125 \pm 0.016 \text{ kcal}\cdot\text{mol}^{-1}$ was measured via solution calorimetry by Taylor and Gardner. <sup>3</sup>					
<b>Heat Capacity and Entropy</b>					
$C_p^\circ$ is based on JANAF curve fits of measurements by adiabatic calorimetry (8–300 K) and by ice calorimetry (354–776 K) as reported by Taylor and Gardner. <sup>3</sup> The sample was estimated as approximately 99.5% BeF <sub>2</sub> . Analyses indicated that the major impurity was about 0.3% oxygen, mainly in the form of absorbed water. Petrographic examination and x-ray diffraction showed the sample to be composed almost completely of quartz-type crystals. The entropy is derived from the smoothed $C_p^\circ$ based on the extrapolation $S^\circ(8\text{ K}) = 0.0065 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . The adopted $C_p^\circ$ above 300 K agrees closely with the relative enthalpy data and shows a remarkable similarity to that of SiO <sub>2</sub> (low quartz).					
<b>Transition Data</b>					
$T_{\text{in}}$ is the value selected by Taylor and Gardner <sup>3</sup> from their relative enthalpy data. $\Delta_{\text{in}}H^\circ$ is the corresponding difference in relative enthalpy from the JANAF curve fits for the two crystalline forms. Levina <sup>4</sup> studied the polymorphism of BeF <sub>2</sub> by observing the peaks in $C_p^\circ$ near the transition temperatures. For low quartz $\rightarrow$ high quartz, Levina's peak began near 438 K, was complete near 503 K, and gave $\Delta_{\text{in}}H^\circ = 0.17 \text{ kcal}\cdot\text{mol}^{-1}$ . Levina found a 2nd transition attributed to a form analogous to tridymite, this began above 670 K, was complete by 740 K, and gave $\Delta_{\text{in}}H^\circ = 0.24 \text{ kcal}\cdot\text{mol}^{-1}$ . There is no evidence for this transition in the relative enthalpy data, so we suspect that its occurrence may be due to impurities in Levina's sample. Levina also found that the cristobalite-like phase transformed in the region 380 to 420 K with $\Delta_{\text{in}}H^\circ = 1.27 \text{ kcal}\cdot\text{mol}^{-1}$ .					
<b>Fusion Data</b>					
Refer to the liquid table for details.					
<b>Sublimation Data</b>					
Refer to the ideal gas table for details.					
<b>References</b>					
<sup>1</sup> V. B. Parker, Nat. Bur. Stand. Report 10004, Chapter 3, p. 58, (January 1, 1969).					
<sup>2</sup> K. L. Churney and G. T. Armstrong, J. Res. Natl. Bur. Stand. 73A, 281 (1969).					
<sup>3</sup> A. R. Taylor and T. Estelle Gardner, U. S. Bur. Mines RI-6664, 15 pp. (1965).					
<sup>4</sup> M. E. Levina, Izv. Vyssh. Ucheb. Zaved., Khim. Teknol. 8 (2), 177 (1965).					

PREVIOUS: June 1964

CURRENT: June 1970

**Beryllium Fluoride (BeF<sub>2</sub>)**

$$S^\circ(298.15\text{ K}) = 23.354 \pm 0.17 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{\text{in}} = 500\text{ K}$$
 (low quartz  $\rightarrow$  high quartz)

$$T_{\text{in}} = 825\text{ K}$$

**Enthalpy of Formation**

$\Delta_f H^\circ$  is the value selected by Parker,<sup>1</sup> based on a thorough review of data for BeF<sub>2</sub>(cr, vitreous, aq) and BeO(cr). Parker's analysis remains essentially unchanged for BeO(cr) and BeF<sub>2</sub>(cr), even though the results for BeF<sub>2</sub>(HF, aq) become more negative by 0.93 kcal·mol<sup>-1</sup> due to JANAF selections for HF(aq). Three values derived for BeF<sub>2</sub>(cr) from pBeF<sub>2</sub>(cr) are changed due to JANAF auxiliary data; these values become  $-246.9$ ,  $-246.0$  and  $-247.2$  for the three paths used by Parker.

The adopted  $\Delta_f H^\circ$  was derived by combination of calorimetric data for Be(cr) + F(g)  $\rightarrow$  BeF<sub>2</sub>(vitreous) and BeF<sub>2</sub>(cr)  $\rightarrow$  BeF<sub>2</sub>(cr). Churney and Armstrong<sup>2</sup> obtained  $\Delta_f H^\circ(298.15\text{ K}) = -244.32 \pm 0.8 \text{ kcal}\cdot\text{mol}^{-1}$  for vitreous BeF<sub>2</sub> by combustion in fluorine of polytetrafluoroethylene and mixtures of Be(cr) with polytetrafluoroethylene.  $\Delta_f H^\circ(298.15\text{ K}, \text{cr} \rightarrow \text{vitreous}) = 1.125 \pm 0.016 \text{ kcal}\cdot\text{mol}^{-1}$  was measured via solution calorimetry by Taylor and Gardner.<sup>3</sup>

**Transition Data**

$T_{\text{in}}$  is the value selected by Taylor and Gardner<sup>3</sup> from their relative enthalpy data.  $\Delta_{\text{in}}H^\circ$  is the corresponding difference in relative enthalpy from the JANAF curve fits for the two crystalline forms. Levina<sup>4</sup> studied the polymorphism of BeF<sub>2</sub> by observing the peaks in  $C_p^\circ$  near the transition temperatures. For low quartz  $\rightarrow$  high quartz, Levina's peak began near 438 K, was complete near 503 K, and gave  $\Delta_{\text{in}}H^\circ = 0.17 \text{ kcal}\cdot\text{mol}^{-1}$ . Levina found a 2nd transition attributed to a form analogous to tridymite, this began above 670 K, was complete by 740 K, and gave  $\Delta_{\text{in}}H^\circ = 0.24 \text{ kcal}\cdot\text{mol}^{-1}$ . There is no evidence for this transition in the relative enthalpy data, so we suspect that its occurrence may be due to impurities in Levina's sample. Levina also found that the cristobalite-like phase transformed in the region 380 to 420 K with  $\Delta_{\text{in}}H^\circ = 1.27 \text{ kcal}\cdot\text{mol}^{-1}$ .

**Fusion Data**

Refer to the liquid table for details.

**Sublimation Data**

Refer to the ideal gas table for details.

**References**

<sup>1</sup>V. B. Parker, Nat. Bur. Stand. Report 10004, Chapter 3, p. 58, (January 1, 1969).

<sup>2</sup>K. L. Churney and G. T. Armstrong, J. Res. Natl. Bur. Stand. 73A, 281 (1969).

<sup>3</sup>A. R. Taylor and T. Estelle Gardner, U. S. Bur. Mines RI-6664, 15 pp. (1965).

<sup>4</sup>M. E. Levina, Izv. Vyssh. Ucheb. Zaved., Khim. Teknol. 8 (2), 177 (1965).

**Beryllium Fluoride (BeF<sub>2</sub>)**Be<sub>1</sub>F<sub>2</sub>(cr)

**Beryllium Fluoride (BeF<sub>2</sub>)****Liquid****Be<sub>1</sub>F<sub>2</sub>(l)**

$$S^\circ(298.15\text{ K}) = [59.920 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}] \\ T_{\text{fus}} = 825\text{ K}$$

**Enthalpy of Formation**

$\Delta_f H^\circ$  is calculated from that of the crystal by means of  $\Delta_f H^\circ = 1.125 \pm 0.016 \text{ kcal}\cdot\text{mol}^{-1}$  for  $\rightarrow \text{BeF}_2(\text{vitreous})$  at 298.15 K. Further details are given in the section on Fusion Data.  $\Delta_f H^\circ(\text{l})$  actually is based on the direct determination of  $\Delta_f H^\circ(\text{vitreous})$  by Churney and Armstrong<sup>1</sup> as discussed on the crystal table.

**Heat Capacity and Entropy**

$C_p^\circ$  is based on a JANAF curve fit of relative enthalpies of Taylor and Gardner<sup>2</sup> for the liquid (828–1183 K) and vitreous (320–473 K) forms of BeF<sub>2</sub>. The combined data yield a normal  $C_p^\circ$  curve and reveal no need for a glass transition. Scatter in the data is somewhat larger than for the crystal, presumably due to minor variations in the vitreous state at the conclusion of each drop.  $S^\circ(298.15\text{ K}, \text{l})$  is calculated from that of the crystal by addition of  $\Delta_{\text{fus}} S^\circ$  and the difference for crystal and liquid of  $S^\circ(825\text{ K}) - S^\circ(298.15\text{ K})$ .

**Fusion Data**

$T_{\text{fus}}$  is the value selected by Taylor and Gardner<sup>2</sup> from their relative enthalpy data. These showed premelting starting near 804 K and complete melting above 828 K. Cooling of the liquid produced the vitreous state.  $T_{\text{fus}}$  has also been reported as 815,<sup>3</sup> 821,<sup>4</sup> 818,<sup>5</sup> and 816 ± 5 K.<sup>6</sup> Solution calorimetry<sup>7</sup> gave  $\Delta_f H^\circ = 1.125 \pm 0.016 \text{ kcal}\cdot\text{mol}^{-1}$  for  $\text{BeF}_2(\text{flow quartz}) \rightarrow \text{BeF}_2(\text{vitreous})$  at 298.15 K. Confirmation of this result came from transposed temperature-drop calorimetry<sup>8</sup> and calorimetric conversion.<sup>9</sup> These gave  $1.1 \pm 0.2$  and  $1.1 \pm 0.5 \text{ kcal}\cdot\text{mol}^{-1}$ , respectively. Combination of  $\Delta_f H^\circ = 1.125$  with JANAF enthalpies yields  $\Delta_{\text{fus}} H^\circ = 1.137 \text{ kcal}\cdot\text{mol}^{-1}$ .

**Vaporization Data**

$T_{\text{vap}}$  is the calculated temperature at which  $\Delta_f G^\circ = 0$  for  $\text{BeF}_2(\text{l}) \rightarrow \text{BeF}_2(\text{g})$ ;  $\Delta_{\text{vap}} H^\circ$  is the corresponding value of  $\Delta_f H^\circ$  at  $T_{\text{vap}}$ . These calculations neglect the presence of dimer, which is assumed to be negligible based on extrapolation of the equations of Belosov.<sup>9</sup> Cantor<sup>10</sup> obtained  $T_{\text{vap}} = 1442\text{ K}$  by extrapolation of his vapor pressures (1146–1372 K).

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<b>M<sub>f</sub> = 47.008986 Beryllium Fluoride (BeF<sub>2</sub>)</b>	
$\Delta_f H^\circ(298.15\text{ K}) = [-1022.048] \text{ kJ}\cdot\text{mol}^{-1}$	
$\Delta_{\text{fus}} H^\circ = 4.757 \text{ kJ}\cdot\text{mol}^{-1}$	
<b>T/K</b>	<b><math>C_p^\circ</math></b>
0	0
100	0
200	49.903
298.15	59.920
300	50.112
400	59.208
500	65.559
600	70.551
700	74.810
800	78.647
825.000	79.538
900	82.228
1000	85.642
1100	88.943
1200	92.165
1300	95.332
1400	98.458
1500	101.550
1600	104.621
1700	107.671
1800	110.709
1900	113.734
2000	116.750
	$S^\circ - [G^\circ - H^\circ(T)/T]$
	$H^\circ - H^\circ(T_r)$
	$\Delta_f H^\circ$
	$\Delta_f G^\circ$
	$\log K_r$

<b>Enthalpy Reference Temperature = <math>T_r = 298.15\text{ K}</math></b>	
<b>Standard State Pressure = <math>p = 0.1 \text{ MPa}</math></b>	
<b>T/K</b>	<b><math>C_p^\circ</math></b>
0	0
100	0
200	0.093
298.15	0.093
300	0.093
400	5.589
500	62.006
600	66.222
700	71.222
800	76.477
825.000	83.066
900	86.956
1000	92.030
1100	96.961
1200	101.745
1300	106.383
1400	110.884
1500	115.253
1600	119.499
1700	123.631
1800	127.555
1900	131.580
2000	135.411
	$J\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
	$\text{kJ}\cdot\text{mol}^{-1}$

Beryllium Fluoride ( $\text{BeF}_2$ ) $M_r = 47.0003986$  $\text{Be}_1\text{F}_2(\text{cr},l)$ 

## CRYSTAL (II-L)-LIQUID

0	to	500 K	crystal, low quartz
500	to	825 K	crystal, high quartz
above		825 K	liquid

Refer to the individual tables for details.

TK	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$			Standard State Pressure = $p^* = 0.1 \text{ MPa}$		
		$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$S^* - (G^* - H(T_r))/T$	$H^* - H(T_r)/T$	$\Delta H^*$	$\Delta G^*$	
0	0	0	0	-8.468	-1024.465	-1024.465	INFINITE
100	21.004	14.253	90.253	-7.550	-1026.493	-1010.881	528.030
200	39.083	35.271	57.702	-4.486	-1026.935	-95.024	259.874
298.15	51.819	53.354	53.354	0.	-1026.754	-979.385	171.584
300	52.028	53.676	53.355	0.096	-1026.746	-979.091	170.475
400	62.522	70.077	55.522	5.822	-1026.081	-943.292	125.793
500	76.048	85.392	59.971	12.710	-1024.661	-947.738	99.009
500,000	76.048	85.392	59.971	12.710	II $\leftrightarrow$ I		
500,000	64.099	85.332	59.971	12.930	TRANSITION		
600	67.446	97.814	63.302	19.508	-1023.604	-932.474	81.179
700	70.793	108.463	70.720	26.420	-1022.636	-917.360	68.454
800	74.140	118.134	76.051	33.666	-1021.495	-902.396	58.970
825,000	74.977	120.428	77.362	35.530	I $\leftrightarrow$ LIQUID		
900	82.228	131.322	81.727	46.354	-1015.054	-885.035	51.540
1000	85.642	142.073	87.724	54.749	-1013.032	-874.028	45.655
1100	88.943	150.391	92.683	63.479	-1010.793	-860.234	40.849
1200	92.165	158.268	97.823	72.535	-1008.342	-846.653	36.854
1300	95.332	165.771	102.763	81.910	-1005.681	-833.286	33.482
1400	98.458	172.950	107.722	91.600	-1002.814	-820.131	30.599
1500	101.350	179.849	112.115	101.600	-999.744	-807.188	28.109
1600	104.621	186.501	116.558	111.909	-1011.010	-793.931	25.919
1700	107.671	192.915	120.862	122.524	-1007.139	-780.481	23.981
1800	110.709	199.175	125.041	133.443	-1002.999	-767.266	22.265
1900	113.734	205.242	129.103	144.665	-998.590	-754.289	20.737
2000	116.750	211.153	133.058	156.189	-993.569	-741.551	19.367

Beryllium Fluoride ( $\text{BeF}_2$ ) $\text{Be}_1\text{F}_2(\text{cr},l)$ Beryllium Fluoride ( $\text{BeF}_2$ )

## CRYSTAL (II-L)-LIQUID

 $\text{Be}_1\text{F}_2(\text{cr},l)$ Beryllium Fluoride ( $\text{BeF}_2$ ) $\text{Be}_1\text{F}_2(\text{cr},l)$ 

PREVIOUS:

CURRENT: June 1970

IDEAL GAS

$$M_r = 47.008986 \text{ Beryllium Fluoride (BeF}_2\text{)}$$

Be<sub>1</sub>F<sub>2</sub>(g)

$$S^\circ(298.15\text{ K}) = [227.56 \pm 1.3] \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$\Delta H^\circ(0\text{ K}) = -796.19 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$$

Enthalpy Reference Temperature =  $T_r = 298.15$  K      Standard State Pressure =  $p^{\circ} = 0.1$  MPa  
 $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$        $\text{kJ}\cdot\text{mol}^{-1}$

Vibrational Frequencies and Degeneracies $v, \text{cm}^{-1}$	Ground State Quantum Weight: 1	$\sigma = 2$
$670(1)$	$345(2)$	$1530(1)$
$u, \text{cm}^{-1}$		

Synthesis of Formation

**Δ*H*<sup>°</sup> of formation.** Δ*H*<sup>°</sup> is calculated from that of the crystal by means of Δ*H*<sup>°</sup>(298.15 K) = 55.15 ± 0.1 kcal mol<sup>-1</sup>. The selected value of Δ<sub>ΔH</sub><sup>°</sup>*H*<sup>°</sup> is an average of those obtained by 3rd law analysis of vapor pressures measured by manometry,<sup>1</sup> torsion effusion,<sup>2</sup> and entrainment.<sup>3-6</sup> Mass-spectrometric data<sup>2</sup> are in reasonable agreement and so is the average of two Knudsen-effusion studies.<sup>6</sup> Several techniques<sup>2-4</sup> were used to show that the amount of dimer in the vapor is negligible up to at least 1000 K. JANAF analyses of the vaporization data are summarized as follows:

- 1 -

**Heat Capacity and Entropy** The bond length and angle are those derived by Akishin *et al.*<sup>11</sup> from electron-diffraction data for the vapor. Linearity of  $\text{BeF}_2$  was confirmed by electric-dipole measurements<sup>12</sup> of the vapor and by infrared studies<sup>13</sup> of matrix-isolated  $\text{BeF}_2$ . Infrared absorptions were found near 30 and 1540  $\text{cm}^{-1}$  in neon matrices, leading to gas-phase estimates of 345 and 1555  $\text{cm}^{-1}$ .<sup>13</sup> The latter absorption was observed<sup>14</sup> at 1520  $\text{cm}^{-1}$  in the infrared spectra of the vapor at 1000°C. We adopt a compromise of 1530  $\text{cm}^{-1}$  and use this value in the valence-force-field calculations.

- ferences

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  5. A. Blaustein, M. A. Greenbaum, J. N. Foster, M. L. Arin and M. Farber, J. Phys. Chem. **69**, 1069 (1965).
  6. M. A. Greenbaum, J. N. Foster, M. L. Arin and M. Farber, J. Phys. Chem. **67**, 36 (1963).
  7. A. M. Essev, G. V. Pozharskaya, E. A. Borisov, An. N. Nesmeyanov and Ya. I. Gerasimov, Zh. Neorg. Khim. **4**, 2192 (1959).

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continued on page 428

Benzillium Elutriate (BoE)

88 E(5)

PREVIOUS: June 1970 (1 atm) CURRENT: June 1970 (1 bar)

## NIST-JANAF THERMOCHEMICAL TABLES

 $\text{Be}_1\text{F}_3\text{Li}_1(\text{cr})$  $M_r = 72.98389$  Lithium Trifluoroberyllate ( $\text{LiBeF}_3$ )

CRYSTAL

$T_{\text{fus}} = [650 \text{ K}]$	$S^{\circ}(298.15 \text{ K}) = 89.24 \pm 4.2 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\Delta_f H^{\circ}(298.15 \text{ K}) = -1651.8 \pm 6.3 \text{ kJ}\cdot\text{mol}^{-1}$	$\Delta_{\text{fus}} H^{\circ} = [27.196] \text{ kJ}\cdot\text{mol}^{-1}$						
Enthalpy of Formation									
Interpolation of the calorimetric enthalpies of mixing of Holm and Kleppa <sup>1</sup> yields $\Delta_f H^{\circ} = -0.56 \pm 0.1 \text{ kcal}\cdot\text{mol}^{-1}$ for $\text{LiF}(\text{l}) + \text{BeF}_3(\text{l}) \rightarrow \text{LiBeF}_3(\text{l})$ at 1135 K. Reduction with the estimated JANAF functions yields $\Delta_f H^{\circ} = -3.07 \pm 1.0 \text{ kcal}\cdot\text{mol}^{-1}$ at 298.15 K for $\text{LiF}(\text{cr}) + \text{BeF}_3(\text{l}) \rightarrow \text{LiBeF}_3(\text{cr})$ , where $\text{BeF}_3(\text{l})$ is the supercooled liquid. $\Delta_f H^{\circ}(298.15 \text{ K})$ for the latter reaction may also be calculated as $-2.77 \pm 0.2 \text{ kcal}\cdot\text{mol}^{-1}$ from the difference of two calorimetric reactions measured by Gross. <sup>2</sup> These results at 298.15 K were $\Delta_f H^{\circ} = -2.28 \pm 0.12 \text{ kcal}\cdot\text{mol}^{-1}$ for $\text{LiF}(\text{cr}) + \text{BeF}_3(\text{cr}) \rightarrow \text{Li}_2\text{BeF}_4(\text{cr})$ and $\Delta_f H^{\circ} = -5.06 \pm 0.06 \text{ kcal}\cdot\text{mol}^{-1}$ for $2\text{LiF}(\text{cr}) + \text{BeF}_3(\text{l}) \rightarrow \text{Li}_2\text{BeF}_4(\text{cr})$ . We adopt the high-temperature results of Holm and Kleppa since the entropy must be calculated by combination of $\Delta_f H^{\circ}$ with $\Delta_f G^{\circ}$ obtained at high temperature.									
Heat Capacity and Entropy	$C_p^{\circ}$ is estimated from $C_p^{\circ}$ of $\text{Li}_2\text{BeF}_4(\text{cr})$ minus $C_p^{\circ}$ of $\text{LiF}(\text{cr})$ . Existing information leads to three values for $S^{\circ}$ at 298.15 K, namely 21.41 $\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ from $\Delta_f G^{\circ}$ and $\Delta_f H^{\circ}$ for mixing of molten $\text{LiF}$ and $\text{BeF}_3$ , 21.33 $\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ from $\text{LiF}(\text{cr})$ and $\text{BeF}_3(\text{cr})$ . We adopt the intermediate value $S^{\circ}(900)$ since it does not involve large contributions from the estimated values of $C_p^{\circ}$ and $\Delta_{\text{fus}} H^{\circ}$ .	$T/K$	$C_p^{\circ}$	$S^{\circ}$	$-(G^{\circ} - H^{\circ}(T))/T$	$H^{\circ} - H^{\circ}(T)/T$	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$	$\log K_t$
Heat Capacity	$C_p^{\circ}$ is estimated from $C_p^{\circ}$ of $\text{Li}_2\text{BeF}_4(\text{cr})$ minus $C_p^{\circ}$ of $\text{LiF}(\text{cr})$ but emphasize that $S^{\circ}(298.15 \text{ K})$ is much more uncertain than indicated by the consistency of the three values. There is less uncertainty in Hitch and Baes' reported emf data and activity coefficients which yield $\Delta_f G^{\circ} = -5.91 \text{ kcal}\cdot\text{mol}^{-1}$ at 900 K for $\text{Li}(\text{l}) + \text{BeF}_3(\text{l}) \rightarrow \text{LiBeF}_3(\text{l})$ . Combining $\Delta_f G^{\circ}$ with $\Delta_f H^{\circ} = -1.05 \text{ kcal}\cdot\text{mol}^{-1}$ , both at 900 K. The corresponding values from the adopted tables are $\Delta_f G^{\circ} = 5.84 \text{ kcal}\cdot\text{mol}^{-1}$ and $S(\text{LiBeF}_3, \text{l}) = 64.46 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , while $S(\text{LiBeF}_3, \text{l}) = 64.38 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ .	200	91.816	89.245	89.245	0.	-1651.843	-1576.273	276.156
Enthalpy of Disproportionation	No transitions are known between room temperature and $T_{\text{fus}}$ , but $\text{LiBeF}_3(\text{cr})$ does disproportionate into $\text{Li}_2\text{BeF}_4(\text{cr})$ and $\text{BeF}_2$ (high quartz). Disproportionation occurs at 553 K according to the latest phase diagrams, <sup>3</sup> or at 573 K according to Roy <i>et al.</i> <sup>4</sup> The adopted tables yield $\Delta_f G^{\circ} = 0$ at 553 K, but this temperature is very sensitive to the value selected for $S^{\circ}$ , which in turn depends on the estimates of $C_p^{\circ}$ and $\Delta_{\text{fus}} H^{\circ}$ .	298.15	92.048	89.813	89.246	0.170	-1651.836	-1575.904	274.372
Fusion Data	Refer to the liquid table for details.	300	104.600	93.013	93.007	10.002	-1651.725	-1550.535	202.474
References	J. L. Holm and O. J. Kleppa, Inorg. Chem., 8, 207 (1969). P. Gross, Fulmer Res. Inst. Report, R-163/22/Jan. 1966 and R-163/18/Dec. 1964, contract AF 61(052)-447. <sup>1</sup> B. F. Hitch and C. F. Baes, Inorg. Chem., 8, 201 (1969); U. S. Atomic Energy Comm., ORNL-4257, 46 pp. (1968). <sup>2</sup> K. A. Romberg <sup>1</sup> , J. Braustein and R. E. Thomas, J. Phys. Chem., 76, 1154 (1972). <sup>3</sup> R. Thoma, H. Insley, H. A. Friedman, and G. M. Hebert, J. Nucl. Materials 27, 166 (1968). <sup>4</sup> D. M. Roy, R. Roy and E. F. Osborn, J. Amer. Ceram. Soc. 37, 300 (1954).	400	117.152	142.702	100.522	21.090	-1653.272	-1525.148	159.331
		500	129.704	165.171	109.450	33.433	-1651.389	-1499.682	130.559
		600	175.801	114.147	40.075	---	CRYSTAL <-> LIQUID	---	---
		700	142.256	186.108	118.921	47.031	-1648.435	-1474.616	110.037
		800	154.808	205.923	128.568	61.884	-1644.389	-1450.048	94.678
		900	167.360	224.881	138.223	77.992	-1639.246	-1426.053	82.766
		1000	179.912	243.164	147.808	93.356	-1632.986	-1402.690	73.269
		1100	192.464	260.900	157.296	113.975	-1625.600	-1380.009	65.531
		1200	205.016	278.185	166.644	133.849	-1617.079	-1358.049	59.114

Lithium Trifluoroberyllate ( $\text{LiBeF}_3$ )

CRYSTAL

$$S^{\circ}(298.15 \text{ K}) = 89.24 \pm 4.2 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{\text{fus}} = [650 \text{ K}]$$

$$\Delta_f H^{\circ}(298.15 \text{ K}) = -1651.8 \pm 6.3 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_{\text{fus}} H^{\circ} = [27.196] \text{ kJ}\cdot\text{mol}^{-1}$$

## Enthalpy of Formation

Interpolation of the calorimetric enthalpies of mixing of Holm and Kleppa<sup>1</sup> yields  $\Delta_f H^{\circ} = -0.56 \pm 0.1 \text{ kcal}\cdot\text{mol}^{-1}$  for  $\text{LiF}(\text{l}) + \text{BeF}_3(\text{l}) \rightarrow \text{LiBeF}_3(\text{l})$  at 1135 K. Reduction with the estimated JANAF functions yields  $\Delta_f H^{\circ} = -3.07 \pm 1.0 \text{ kcal}\cdot\text{mol}^{-1}$  at 298.15 K for  $\text{LiF}(\text{cr}) + \text{BeF}_3(\text{l}) \rightarrow \text{LiBeF}_3(\text{cr})$ , where  $\text{BeF}_3(\text{l})$  is the supercooled liquid.  $\Delta_f H^{\circ}(298.15 \text{ K})$  for the latter reaction may also be calculated as  $-2.77 \pm 0.2 \text{ kcal}\cdot\text{mol}^{-1}$  from the difference of two calorimetric reactions measured by Gross.<sup>2</sup> These results at 298.15 K were  $\Delta_f H^{\circ} = -2.28 \pm 0.12 \text{ kcal}\cdot\text{mol}^{-1}$  for  $\text{LiF}(\text{cr}) + \text{BeF}_3(\text{cr}) \rightarrow \text{Li}_2\text{BeF}_4(\text{cr})$  and  $\Delta_f H^{\circ} = -5.06 \pm 0.06 \text{ kcal}\cdot\text{mol}^{-1}$  for  $2\text{LiF}(\text{cr}) + \text{BeF}_3(\text{l}) \rightarrow \text{Li}_2\text{BeF}_4(\text{cr})$ . We adopt the high-temperature results of Holm and Kleppa since the entropy must be calculated by combination of  $\Delta_f H^{\circ}$  with  $\Delta_f G^{\circ}$  obtained at high temperature.

## Heat Capacity and Entropy

$C_p^{\circ}$  is estimated from  $C_p^{\circ}$  of  $\text{Li}_2\text{BeF}_4(\text{cr})$  minus  $C_p^{\circ}$  of  $\text{LiF}(\text{cr})$  but emphasize that  $S^{\circ}(298.15 \text{ K})$  is much more uncertain than indicated by the consistency of the three values. There is less uncertainty in Hitch and Baes' reported emf data and activity coefficients which yield  $\Delta_f G^{\circ} = -5.91 \text{ kcal}\cdot\text{mol}^{-1}$  at 900 K for  $\text{Li}(\text{l}) + \text{BeF}_3(\text{l}) \rightarrow \text{LiBeF}_3(\text{l})$ . Combining  $\Delta_f G^{\circ}$  with  $\Delta_f H^{\circ} = -1.05 \text{ kcal}\cdot\text{mol}^{-1}$ , both at 900 K. The corresponding values from the adopted tables are  $\Delta_f G^{\circ} = 5.84 \text{ kcal}\cdot\text{mol}^{-1}$  and  $S(\text{LiBeF}_3, \text{l}) = 64.46 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , while  $S(\text{LiBeF}_3, \text{l}) = 64.38 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ .

## Disproportionation Data

No transitions are known between room temperature and  $T_{\text{fus}}$ , but  $\text{LiBeF}_3(\text{cr})$  does disproportionate into  $\text{Li}_2\text{BeF}_4(\text{cr})$  and  $\text{BeF}_2$  (high quartz). Disproportionation occurs at 553 K according to the latest phase diagrams,<sup>3</sup> or at 573 K according to Roy *et al.*<sup>4</sup> The adopted tables yield  $\Delta_f G^{\circ} = 0$  at 553 K, but this temperature is very sensitive to the value selected for  $S^{\circ}$ , which in turn depends on the estimates of  $C_p^{\circ}$  and  $\Delta_{\text{fus}} H^{\circ}$ .

## Fusion Data

Refer to the liquid table for details.

## References

- <sup>1</sup>J. L. Holm and O. J. Kleppa, Inorg. Chem., 8, 207 (1969).
- <sup>2</sup>P. Gross, Fulmer Res. Inst. Report, R-163/22/Jan. 1966 and R-163/18/Dec. 1964, contract AF 61(052)-447.
- <sup>3</sup>B. F. Hitch and C. F. Baes, Inorg. Chem., 8, 201 (1969); U. S. Atomic Energy Comm., ORNL-4257, 46 pp. (1968).
- <sup>4</sup>K. A. Romberg<sup>1</sup>, J. Braustein and R. E. Thomas, J. Phys. Chem., 76, 1154 (1972).
- <sup>5</sup>R. Thoma, H. Insley, H. A. Friedman, and G. M. Hebert, J. Nucl. Materials 27, 166 (1968).
- <sup>6</sup>D. M. Roy, R. Roy and E. F. Osborn, J. Amer. Ceram. Soc. 37, 300 (1954).

Lithium Trifluoroberyllate (LiBeF<sub>3</sub>)

## LIQUID

Be<sub>1</sub>F<sub>3</sub>Li<sub>1</sub>(I)

$$S^{\circ}(298.15\text{ K}) = [111.681] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{\text{fus}} = [650] \text{ K}$$

## Enthalpy of Formation

$\Delta_f H^{\circ}$  is calculated from that of the crystal by addition of  $\Delta_{\text{fus}} H^{\circ}$  and the difference in enthalpy,  $H^{\circ}(650\text{ K}) - H^{\circ}(298.15\text{ K})$ , between the crystal and liquid. Note that the result is based on direct measurements of the enthalpy of mixing of molten LiF and BeF<sub>2</sub> at 1135 K.<sup>1</sup>

## Heat Capacity and Entropy

$C_p^{\circ}$  is estimated on the basis of 7.6 cal·K<sup>-1</sup>·mol<sup>-1</sup> by comparison with the liquid phases of LiF, BeF<sub>2</sub> and Li<sub>2</sub>BeF<sub>4</sub>. A glass transition is assumed at 400 K and below this temperature  $C_p^{\circ}$  is obtained from that of the crystal. The entropy is calculated in a manner analogous to that used for  $\Delta_f H^{\circ}$ . Note that the resulting value of  $S^{\circ}$  (900 K) differs by only 0.08 cal·K<sup>-1</sup>·mol<sup>-1</sup> from that based on measurements of  $\Delta_f H^{\circ}$  (1135 K)<sup>1</sup> and  $\Delta_G^{\circ}$  (900 K)<sup>2</sup> for mixing of molten LiF and BeF<sub>2</sub>.

## Fusion Data

The composition corresponding to LiBeF<sub>3</sub> melts incongruently,<sup>1</sup> starting with the eutectic composition of 53 mole percent BeF<sub>2</sub> at 636.6  $\pm$  0.5 K and finishing at a liquidus temperature near 633 K. Just below the melting region, the solid consists of an equimolar mixture of Li<sub>2</sub>BeF<sub>4</sub>(cr) and BeF<sub>2</sub>(high quartz). We arbitrarily adopt 650 K as the hypothetical, congruent melting point of metastable LiBeF<sub>3</sub>. We estimate  $\Delta_{\text{fus}} H^{\circ}$  on the basis of  $\Delta_{\text{fus}} S^{\circ} = 2.0 \text{ cal}\cdot\text{K}^{-1}\cdot\text{g}^{-1}$  by comparison with Li<sub>2</sub>BeF<sub>4</sub>.

## Vaporization Data

Mass-spectrometric data<sup>4,5</sup> for the LiF–BeF<sub>2</sub> system suggest that the vapor consists mainly of BeF<sub>3</sub>(g), some LiBeF<sub>3</sub>(g), and traces of other molecules.

## References

- <sup>1</sup>J. L. Holm and O. J. Kleppa, Inorg. Chem. 8, 207 (1969).
- <sup>2</sup>B. F. Hitch and C. F. Baes, Inorg. Chem. 8, 201 (1969); U. S. Atomic Energy Comm., ORNL-4257, 46 pp. (1968).
- <sup>3</sup>K. A. Romberger, J. Braunsien and R. E. Thoma, J. Phys. Chem., 76, 1154 (1972).
- <sup>4</sup>A. Buchler and J. L. Stauffer, Thermodynamics, Proc. Symp., Vienna, 1965, I, 271; Int. At. Energy Agency, Vienna, (1966).
- <sup>5</sup>J. Berkowitz, and W. A. Chupka, Ann. New York Acad. Sci. 79, Art. 11, 1073 (1960).

M<sub>r</sub> = 72.948389Be<sub>1</sub>F<sub>3</sub>Li<sub>1</sub>(I)

T/K	$C_p^{\circ}$	$S^{\circ}$	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$			Standard State Pressure = $p^{\circ} = 0.1 \text{ MPa}$		
			$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$-\left[G^{\circ} - H^{\circ}(T)\right]/T$	$\text{kJ}\cdot\text{mol}^{-1}$	$H^{\circ} - H^{\circ}(T_r)$	$\Delta_H^{\circ}$	$\Delta_G^{\circ}$
0								
100								
200								
298.15	91.816	111.681	111.681	0	0	-1634.323	-1565.442	274.259
300	92.048	112.449	111.683	0.170	0.170	-1634.315	-1565.014	272.493
400	104.600	140.449	115.443	10.002	10.002	-1633.755	-1541.988	201.363
400.001	104.600	140.449	115.443	10.003	10.003	GLASS	GLASS	GLASS
400.001	138.992	140.449	115.443	10.003	10.003	—> LIQUID	—> LIQUID	—> LIQUID
500	158.992	175.927	124.124	25.902	25.902	-1630.939	-1519.428	158.734
600	158.992	204.915	135.247	41.801	41.801	-1625.501	-1497.640	130.381
650.000	158.992	217.6541	141.102	49.750	49.750	—> CRYSTAL	—> CRYSTAL	—> CRYSTAL
700	158.992	229.423	146.995	57.700	57.700	-1620.246	-1476.748	110.196
800	250.654	158.635	73.599	1615.154	1615.154	-1456.597	95.106	
900	269.380	169.938	89.498	1610.219	1610.219	-1437.076	83.406	
1000	286.132	180.734	105.398	1605.424	1605.424	-1418.096	74.074	
1100	301.285	191.015	121.297	1600.757	1600.757	-1399.590	66.461	
1200	315.119	200.789	137.196	1596.211	1596.211	-1381.503	60.135	
1300	327.246	210.080	153.095	1591.792	1591.792	-1363.792	54.798	
1400	339.528	218.918	168.994	1587.468	1587.468	-1346.417	50.215	
1500	350.997	227.335	184.894	1583.263	1583.263	-1329.346	46.292	
1600	360.859	235.163	200.793	1593.702	1593.702	-1312.027	42.833	
1700	370.997	243.032	216.692	1734.546	1734.546	-1287.380	39.536	
1800	379.985	250.168	232.591	1729.437	1729.437	-1261.224	36.600	
1900	388.181	257.197	248.490	1724.368	1724.368	-1235.351	33.962	
2000	396.337	264.142	264.390	1719.337	1719.337	-1209.743	31.595	

PREVIOUS:

Lithium Trifluoroberyllate (LiBeF<sub>3</sub>)Be<sub>1</sub>F<sub>3</sub>Li<sub>1</sub>(I)

CURRENT: December 1971

Lithium Trifluoroberyllate ( $\text{LiBeF}_3$ )

## CRYSTAL-LIQUID

0 to 650 K  
above 650 K  
crystal  
liquid

Refer to the individual tables for details.

 $M_r = 72.948389$  Lithium Trifluoroberyllate ( $\text{LiBeF}_3$ ) $\text{Be}_1\text{F}_3\text{Li}_1(\text{cr},\text{l})$ 

T/K	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^* = 0.1 \text{ MPa}$	
		$S^* - [G^* - H^*(T_r)]/T$	$H^* - H^*(T_r)$	$\Delta_f H^*$	$\Delta_f G^*$
0					
100					
200					
298.15	91.816	89.245	89.245	0.	-1651.843
300	92.048	89.813	89.246	0.170	-1651.836
400	104.600	118.013	93.007	10.092	-1651.275
500	117.152	142.702	100.522	21.090	-1651.272
600	129.704	165.171	109.450	33.433	-1651.389
650.000	135.980	175.801	114.147	40.075	-1499.682
650.000	138.992	217.641	114.147	61.271	— CRYSTAL $\rightleftharpoons$ LIQUID —
700	138.992	229.423	121.965	75.221	-1620.246
800	158.992	250.654	136.754	91.120	-1615.154
900	158.992	269.380	150.470	107.019	-1610.219
1000	158.992	286.132	163.211	122.918	-1605.424
1100	158.992	301.285	175.088	138.817	-1600.757
1200	158.992	315.119	186.189	154.717	-1596.590
1300	158.992	327.846	196.563	170.616	-1591.783
1400	158.992	339.628	206.403	186.315	-1587.468
1500	158.992	350.597	215.655	202.414	-1583.263
1600	158.992	360.859	224.413	218.313	-1593.702
1700	158.992	370.497	232.725	234.213	-1734.546
1800	158.992	379.585	240.634	250.112	-1729.437
1900	158.992	388.181	248.176	268.011	-1723.368
2000	158.992	396.337	255.382	281.910	-1719.337

 $\text{Be}_1\text{F}_3\text{Li}_1(\text{cr},\text{l})$ 

T/K	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^* = 0.1 \text{ MPa}$	
		$S^* - [G^* - H^*(T_r)]/T$	$H^* - H^*(T_r)$	$\Delta_f H^*$	$\Delta_f G^*$
0					
100					
200					
298.15	91.816	89.245	89.245	0.170	-1575.804
300	92.048	89.813	89.246	0.170	-1575.804
400	104.600	118.013	93.007	10.092	-1550.555
500	117.152	142.702	100.522	21.090	-1525.148
600	129.704	165.171	109.450	33.433	-1499.682
650.000	135.980	175.801	114.147	40.075	— CRYSTAL $\rightleftharpoons$ LIQUID —
650.000	138.992	217.641	114.147	61.271	-1476.748
700	138.992	229.423	121.965	75.221	-1620.246
800	158.992	250.654	136.754	91.120	-1615.154
900	158.992	269.380	150.470	107.019	-1610.219
1000	158.992	286.132	163.211	122.918	-1605.424
1100	158.992	301.285	175.088	138.817	-1600.757
1200	158.992	315.119	186.189	154.717	-1596.590
1300	158.992	327.846	196.563	170.616	-1591.783
1400	158.992	339.628	206.403	186.315	-1587.468
1500	158.992	350.597	215.655	202.414	-1583.263
1600	158.992	360.859	224.413	218.313	-1593.702
1700	158.992	370.497	232.725	234.213	-1734.546
1800	158.992	379.585	240.634	250.112	-1729.437
1900	158.992	388.181	248.176	268.011	-1723.368
2000	158.992	396.337	255.382	281.910	-1719.337

## IDEAL GAS

Lithium Trifluoroberyllate (LiBeF<sub>3</sub>)

$$S^*(298.15 \text{ K}) = [267.42] J \cdot K^{-1} \cdot mol^{-1}$$

$$\Delta_f H^\circ(0 \text{ K}) = -880 \text{ kJ} \cdot mol^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = -887 \text{ kJ} \cdot mol^{-1}$$

Vibrational Frequencies and Degeneracies v, cm <sup>-1</sup>	
[1530] (1)	[485] (2)
[820] (2)	[800] (3)
[700] (1)	

Point Group: [C<sub>nv</sub>] σ = [3]

Bond Distances. Be-F = [1.40] Å; Li-Be = [1.209] Å; Li-F = [1.85] Å

Bond Angles. F-Be F = [120]<sup>o</sup>. Li-Be-F = [90]<sup>o</sup>Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [2.1635 × 10<sup>-11</sup>] g<sup>3</sup>·cm<sup>6</sup>

## Enthalpy of Formation

$\Delta_f H^\circ(298.15 \text{ K})$  is calculated from  $\Delta_f H^\circ(900 \text{ K}) = 53 \text{ kcal mol}^{-1}$  for the reaction LiF(g) + BeF<sub>3</sub>(g) = LiBeF<sub>3</sub>(g) reported by Hildenbrand, et al.<sup>1</sup>

## Heat Capacity and Entropy

The molecular structure was assumed to be pyramidal with Li atom at the top and BeF<sub>3</sub> located at the bottom. Beryllium atom was taken at the center of the equilateral triangle formed by the three F atoms. The Be-F distance was estimated from that of BeF<sub>3</sub>. The bond distance of Li-F was taken from Porter and Zeller.<sup>2</sup> Vibrational frequencies were estimated by comparison with related fluorides. The principal moments of inertia are: I<sub>A</sub> = I<sub>B</sub> = 10.7996 × 10<sup>-19</sup> and I<sub>C</sub> = 18.5503 × 10<sup>-19</sup> g·cm<sup>2</sup>.

## References

- <sup>1</sup>D. L. Hildenbrand, et al., Aeronutronic Division of Ford Motor Co., Publication No. U-1734, (June 1952).  
<sup>2</sup>R. F. Porter and E. E. Zeller, J. Chem. Phys., 33, 858 (1960).

Lithium Trifluoroberyllate (LiBeF<sub>3</sub>)Be<sub>1</sub>F<sub>3</sub>Li<sub>1</sub>(g)

	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K				Standard State Pressure = p = 0.1 MPa				
	T/K	C <sup>*</sup>	S <sup>*</sup>	[G <sup>*</sup> -H <sup>*</sup> (T <sub>r</sub> )]/T	H <sup>*</sup> -H <sup>*</sup> (T <sub>r</sub> )	Δ <sub>r</sub> H <sup>*</sup>	kJ/mol <sup>-1</sup>	Δ <sub>r</sub> G <sup>*</sup>	log K <sub>s</sub>
0	0	0	0	INFINITE	-12.459	-879.655	-879.655	INFINITE	
100	34.100	219.860	31.078	-981.523	-876.878	-876.878	-876.878	480.034	
200	45.467	246.303	272.513	-5.242	-884.166	-871.430	-871.430	227.592	
250	53.629	257.324	268.384	-2.765	-885.662	-868.072	-868.072	181.374	
298.15	61.090	267.419	267.419	0.	-887.008	-864.560	-864.560	151.467	
300	61.360	267.798	267.420	0.113	-887.038	-864.421	-864.421	150.509	
350	68.105	277.777	268.193	3.354	-889.341	-860.545	-860.545	128.429	
400	73.789	287.253	269.988	6.906	-890.536	-865.492	-865.492	111.846	
450	78.517	295.226	272.410	10.171	-890.567	-852.292	-852.292	98.932	
500	82.442	304.708	275.219	14.744	-891.782	-847.661	-847.661	88.555	
600	88.434	320.301	281.458	23.306	-896.681	-838.052	-838.052	72.559	
700	92.663	334.269	288.022	32.373	-898.238	-828.152	-828.152	61.797	
800	95.714	346.553	294.603	41.800	-899.638	-818.041	-818.041	53.413	
900	97.986	358.264	301.052	51.491	-900.912	-807.764	-807.764	46.881	
1000	99.100	368.681	307.302	61.379	-902.128	-797.349	-797.349	41.649	
1100	101.024	378.248	313.323	71.418	-903.322	-786.813	-786.813	37.363	
1200	102.064	387.085	319.106	81.574	-904.518	-776.169	-776.169	33.786	
1300	102.995	393.288	324.655	91.324	-905.740	-765.424	-765.424	30.755	
1400	103.568	402.939	329.976	102.148	-907.000	-754.583	-754.583	28.154	
1500	104.121	410.104	335.082	112.533	-908.309	-743.651	-743.651	25.896	
1600	104.579	416.339	339.983	122.569	-914.211	-732.104	-732.104	23.904	
1700	104.963	423.191	344.693	133.447	-910.477	-710.477	-710.477	21.904	
1800	105.288	429.200	349.222	143.960	-910.753	-691.847	-691.847	20.077	
1900	105.566	434.590	353.583	154.503	-911.034	-670.789	-670.789	18.441	
2000	105.804	440.321	357.785	165.071	-911.340	-649.716	-649.716	16.069	
2100	106.011	445.488	361.839	175.662	-911.650	-628.627	-628.627	15.636	
2200	106.190	450.424	365.755	186.273	-912.970	-607.523	-607.523	14.424	
2300	106.348	453.148	369.539	196.900	-912.298	-586.404	-586.404	13.303	
2400	106.487	459.677	372.201	207.542	-912.631	-565.221	-565.221	12.303	
2500	106.610	464.027	376.748	218.197	-912.967	-544.125	-544.125	11.369	
2600	106.719	468.210	380.186	228.863	-913.303	-522.964	-522.964	10.506	
2700	106.817	472.140	383.521	239.540	-913.638	-501.791	-501.791	9.708	
2800	106.905	476.126	386.596	250.226	-914.926	-482.383	-482.383	8.850	
2900	106.984	479.879	389.906	260.921	-916.226	-462.591	-462.591	7.972	
3000	107.055	483.507	392.966	271.623	-916.525	-440.825	-440.825	7.153	
3100	107.120	487.018	395.943	282.332	-917.821	-420.542	-420.542	6.388	
3200	107.179	490.420	398.943	293.047	-918.135	-400.369	-400.369	5.670	
3300	107.232	493.719	401.668	303.767	-918.456	-380.166	-380.166	4.997	
3400	107.281	496.921	404.423	314.493	-918.776	-360.016	-360.016	4.363	
3500	107.326	500.032	407.111	325.223	-919.295	-342.377	-342.377	3.767	
3600	107.368	503.596	409.734	345.938	-919.417	-321.095	-321.095	3.203	
3700	107.406	508.653	412.296	346.597	-919.527	-301.824	-301.824	2.671	
3800	107.441	510.863	414.800	357.439	-919.630	-281.554	-281.554	2.216	
3900	107.473	511.654	417.248	368.185	-919.733	-261.284	-261.284	1.888	
4000	107.503	514.375	419.642	378.934	-919.837	-241.027	-241.027	1.235	
4100	107.531	517.030	421.985	389.685	-920.929	-221.769	-221.769	0.803	
4200	107.557	519.622	424.279	400.940	-931.040	-201.509	-201.509	0.393	
4300	107.581	522.153	426.526	411.197	-931.157	-181.174	-181.174	0.092	
4400	107.604	524.626	428.727	421.956	-931.264	-161.609	-161.609	0.022	
4500	107.625	527.045	430.885	432.718	-931.374	-142.037	-142.037	-0.372	
5000	107.712	538.389	441.078	486.533	-934.553	-134.677	-134.677	-2.293	
5100	107.727	540.522	443.007	497.325	-934.641	-125.842	-125.842	-2.569	
5200	107.741	542.614	444.903	508.099	-934.732	-114.560	-114.560	-2.834	
5300	107.754	544.667	446.766	518.873	-934.828	-104.934	-104.934	-3.089	
5400	107.766	546.681	448.598	529.649	-934.924	-94.464	-94.464	-3.335	
5500	107.777	548.638	450.399	540.426	-935.020	-84.057	-84.057	-3.571	
5600	107.788	550.600	452.171	551.205	-935.113	-74.776	-74.776	-3.799	
5700	107.799	552.578	453.915	561.384	-935.204	-65.438	-65.438	-4.019	
5800	107.808	554.583	455.631	572.764	-935.293	-56.202	-56.202	-4.231	
5900	107.818	556.226	457.320	573.827	-935.382	-47.101	-47.101	-4.436	
6000	107.827	558.038	458.984	594.328	-935.466	-38.316	-38.316	-4.634	

CURRENT: December 1962 (1 atm)  
PREVIOUS: December 1962 (1 atm)Lithium Trifluoroberyllate (LiBeF<sub>3</sub>)Be<sub>1</sub>F<sub>3</sub>Li<sub>1</sub>(g)

Lithium Tetrafluoroberyllate ( $\text{Li}_2\text{BeF}_4$ )

## CRYSTAL

 $M_r = 98.887792$  Lithium Tetrafluoroberyllate ( $\text{LiBeF}_4$ ) $\text{Be}_1\text{F}_4\text{Li}_2(\text{cr})$ 

$\Delta_f H^\circ(0 \text{ K}) = \text{Unknown}$	$\Delta_f H^\circ(298.15 \text{ K}) = 2.1 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\Delta_{hs} H^\circ = -2273.6 \pm 5.0 \text{ kJ}\cdot\text{mol}^{-1}$	$\Delta_{hs} H^\circ = 43.995 \pm 2.09 \text{ kJ}\cdot\text{mol}^{-1}$			
$T_{\text{fus}} = 732.2 \pm 0.2 \text{ K}$						
<b>Enthalpy of Formation</b>						
<p>Interpolation of the calorimetric enthalpies of mixing of Holm and Kleppa<sup>1</sup> yields <math>\Delta_f H^\circ = -3.2 \pm 0.1 \text{ kcal}\cdot\text{mol}^{-1}</math> for <math>2\text{LiF}(\text{l}) + \text{BeF}_4(\text{l}) \rightarrow \text{Li}_2\text{BeF}_4(\text{l})</math> at 1135 K. Reduction with the estimated JANAF functions yields <math>\Delta_f H^\circ = -4.24 \pm 0.02 \text{ kcal}\cdot\text{mol}^{-1}</math> at 298.15 K for <math>2\text{LiF}(\text{cr}) + \text{BeF}_4(\text{l}) \rightarrow \text{Li}_2\text{BeF}_4(\text{cr})</math>, where <math>\text{BeF}_4(\text{l})</math> is the supercooled liquid. Gross<sup>2</sup> studied the latter reaction calorimetrically and obtained <math>\Delta_f H^\circ = -5.05 \pm 0.06 \text{ kcal}\cdot\text{mol}^{-1}</math> at 298.15 K. The difference of 0.8 <math>\text{kcal}\cdot\text{mol}^{-1}</math> between the two results is greater than the combined uncertainties but probably is not unreasonable in this case. We adopt the high-temperature results of Holm and Kleppa since the entropy must be calculated by combination of <math>\Delta_f H^\circ</math> with <math>\Delta_f G^\circ</math> obtained at high temperature.</p>						
$T/K$	$C_p^\circ$	$S^\circ$	$-\left[G^\circ - f(T)\right]/T$			
0						
100						
200	135.269	130.583	0.			
298.15	135.269	130.583	-2273.586			
300	135.220	130.585	-2273.573			
400	150.457	172.453	-2272.755			
500	165.552	146.947	-2277.665			
600	180.247	159.724	-2275.563			
700	195.184	173.152	-2277.139			
732.200	199.995	267.997	-2032.747			
732.200	199.995	276.882	172.553			
— CRYSTAL <--> LIQUID —						
800	210.100	295.034	186.715			
900	225.004	320.641	108.411			
1000	239.911	345.119	213.462			
1100	254.819	368.684	226.509			
1200	269.729	391.495	182.620			
1300	284.640	413.674	239.312			
1400	299.554	435.314	264.208			
1500	314.469	456.490	276.323			

## Transition Data

$\text{Li}_2\text{BeF}_4$  has a hexagonal unit cell (space group R $\bar{3}$ ) isotropic with phenacite.<sup>6</sup> This structure shows no phase transitions between room temperature and  $T_{\text{fus}}$ ,<sup>3,7</sup> but exposure to traces of moisture at elevated temperatures causes decomposition to  $\text{LiF}$  and  $\text{BeO}$ .<sup>7,8</sup> Metastable forms have been reported<sup>4</sup> but not confirmed or identified.

## Fusion Data

New electrochemical measurements<sup>9</sup> of the liquidus in the  $\text{LiF}-\text{BeF}_4$  system show that  $\text{LiBeF}_4$  melts congruently at  $459.1 \pm 0.2^\circ\text{C}$  with the eutectic point at  $458.9 \pm 0.2^\circ\text{C}$  and 32.8 mole percent  $\text{BeF}_4$ . The close proximity of the eutectic explains previous conflicting reports of incongruent<sup>1</sup> and congruent<sup>4,10</sup> melting. We adopt  $T_{\text{fus}} = 732.2 \pm 0.2 \text{ K}$  and derive  $\Delta_{hs} H^\circ = 10.515 \text{ kcal}\cdot\text{mol}^{-1}$  from the difference in smoothed enthalpies for liquid and crystal.<sup>3</sup> The uncertainty estimated for  $\Delta_{hs} H^\circ$  emphasized the nature of the premelting corrections.

## References

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Lithium Tetrafluoroberyllate ( $\text{Li}_2\text{BeF}_4$ )

## LIQUID

Lithium Tetrafluoroberyllate ( $\text{Li}_2\text{BeF}_4$ )

$$\Delta_fH^\circ(298.15 \text{ K}) = [171.395] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{fus}} = 732.2 \pm 0.2 \text{ K}$$

## Enthalpy of Formation

$\Delta_fH^\circ$  is calculated from that of the crystal by addition of  $\Delta_{\text{vap}}H^\circ$  and the difference in enthalpy of mixing of molten LiF and  $\text{BeF}_2$  at 1135 K.<sup>1</sup> Note that the result is based on direct measurements of the enthalpy of mixing of crystal and liquid. Note that the result is based on direct measurements of the enthalpy of mixing of molten LiF and  $\text{BeF}_2$  at 1135 K.<sup>1</sup>

## Heat Capacity and Entropy

The constant  $C_p^*$  is derived from enthalpy data (732.2 K) of Douglas and Payne.<sup>2</sup> A glass transition is assumed at 500 K and below this temperature  $C_p^*$  is obtained from that of the crystal. The entropy is calculated in a manner analogous to that used for  $\Delta_fH^\circ$ . Note that the result is based on measurements of  $\Delta_fH^\circ(1135 \text{ K})$  and  $\Delta_fG^\circ(900 \text{ K})$ <sup>3</sup> for mixing of molten LiF and  $\text{BeF}_2$ .

## Fusion Data

Refer to the crystal table for details.

## Vaporization Data

Mass spectra of vapor effusing from twin-crucible Knudsen cells<sup>4</sup> suggest that the vapor consists of  $\text{BeF}_2$ ,  $\text{LiBeF}_3$  and traces of other molecules.

## References

- J. L. Holm and O. J. Kleppa, Inorg. Chem. 8, 207 (1969).
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		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$				Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$			
		$T/K$	$C_p^*/\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$	$S^\circ/\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$	$-[G^\circ - H^\circ(T)]/T$	$H^\circ - H^\circ(T_r)/T$	$\Delta_fH^\circ/\text{kJ} \cdot \text{mol}^{-1}$	$\Delta_fG^\circ/\text{kJ} \cdot \text{mol}^{-1}$	$\log K_r$
0		100	165.552	248.440	187.759	30.341	-2241.068	-2151.088	
298.15		135.269	171.395	171.395	0.				376.862
300		135.520	172.232	171.397	0.250	-2241.055	-2150.530	374.441	
400		150.457	213.265	176.891	14.550	-2240.238	-2120.372	276.905	
500		165.352	248.440	187.759	30.340	-2245.147	-2090.036	218.345	
500.001		165.552	248.440	187.759	30.341	-2237.119	-2229.255	GLASS $\leftarrow \rightarrow$ LIQUID	
500.001		232.086	248.440	187.759	30.341	-2239.255	-2039.771	CRYSTAL $\leftarrow \rightarrow$ LIQUID	
600		232.086	290.754	201.506	53.549	-2237.119	-2039.771	179.319	
700		232.086	326.530	216.877	76.758	-2239.255	-2030.837	151.543	
732.200		232.086	336.968	221.930	84.231	-2239.255	-2030.837		
800		232.086	357.521	232.563	99.966	-2231.555	-2031.019	130.784	
900		232.086	384.837	247.996	123.175	-2214.039	-1971.019	114.693	
1000		232.086	409.310	262.926	146.384	-2196.635	-1950.122	101.864	
1100		232.086	431.430	277.255	169.592	-2199.420	-1924.820	91.402	
1200		232.086	451.624	290.957	192.801	-2192.313	-1900.171	82.712	
1300		232.086	470.201	304.040	216.010	-2185.313	-1876.110	75.383	
1400		232.086	487.400	316.530	259.218	-2178.470	-1852.382	69.121	
1500		232.086	503.413	328.461	262.427	-2171.718	-1829.240	63.710	
1600		232.086	518.391	339.869	285.635	-2179.611	-1806.420	58.974	
1700		232.086	532.461	350.788	308.844	-2463.146	-1768.956	54.353	
1800		232.086	545.727	361.253	332.053	-2454.737	-1728.364	50.156	
1900		232.086	558.275	371.296	355.261	-2446.377	-1688.238	46.413	
2000		232.086	570.180	380.945	378.470	-2438.061	-1648.551	43.036	
2100		232.086	581.503	390.228	401.679	-2429.783	-1602.280	40.029	
2200		232.086	592.300	399.169	413.887	-2421.540	-1570.402	37.286	
2300		232.086	602.617	407.792	424.325	-1531.897	-1493.750	34.790	
2400		232.086	612.494	416.117	471.305	-2405.134	-1493.750	32.511	
2500		232.086	621.968	424.163	494.513	-2396.963	-1455.944	30.420	

Lithium Tetrafluoroberyllate ( $\text{Li}_2\text{BeF}_4$ )

## CRYSTAL-LIQUID

0 to 732.2 K  
above 732.2 K

crystal  
liquid

Refer to the individual tables for details.

 $M_r = 98.887792$  Lithium Tetrafluoroberyllate ( $\text{Li}_2\text{BeF}_4$ ) $\text{Be}_1\text{F}_4\text{Li}_2(\text{cr},\text{l})$ 

$T/K$	$C_p^*$	$\text{Enthalpy Reference Temperature} = T_r = 298.15 \text{ K}$		$\text{Standard State Pressure} = p^* = 0.1 \text{ MPa}$		
		$\text{[K}^\circ\text{mol}^{-1}]$	$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\text{kJ}\cdot\text{mol}^{-1}$	$\Delta G^\circ$
0						
100						
200	135.269	130.383	130.383	0.	-2273.586	-2171.438
300	135.520	131.420	130.585	0.250	-2273.573	-2170.804
400	150.457	172.453	156.079	14.550	-2272.755	-2136.665
500	163.352	207.627	146.547	30.340	-2271.663	-2102.147
600	180.247	239.090	159.724	47.620	-2275.565	-2067.220
700	195.184	267.997	173.152	66.391	-2272.139	-2032.747
722.200	276.382	177.519	72.753		CRYSTAL $\longleftrightarrow$ LIQUID TRANSITION	
732.200	232.086	177.519	116.748		CRYSTAL $\longleftrightarrow$ LIQUID TRANSITION	
800	232.086	157.521	191.917	132.484	-2221.555	-2003.019
900	232.086	149.310	211.866	211.866	-2214.029	-1976.156
1000	232.086	409.310	230.409	178.901	-2206.635	-1950.122
1100	232.086	431.430	247.694	202.110	-2199.420	-1924.820
1200	232.086	451.524	265.859	225.318	-2192.313	-1900.171
1300	232.086	470.201	279.026	248.527	-2185.333	-1876.110
1400	232.086	487.400	293.304	271.736	-2178.470	-1852.582
1500	232.086	503.413	308.783	294.944	-2171.718	-1829.540
1600	232.086	518.391	319.546	318.153	-2179.611	-1806.420
1700	232.086	532.461	331.060	341.361	-2463.146	58.974
1800	232.086	545.727	343.188	364.570	-2454.737	-1768.936
1900	232.086	558.275	354.181	387.779	-2446.377	-1728.364
2000	232.086	570.180	364.686	410.987	-2438.061	-1688.238
2100	232.086	581.503	374.743	434.196	-2429.783	-1648.551
2200	232.086	592.300	384.389	457.405	-2421.540	-1609.280
2300	232.086	602.617	393.654	480.613	-2413.325	-1531.897
2400	232.086	612.494	402.568	503.822	-2405.134	-1493.750
2500	232.086	621.968	411.156	527.031	-2396.963	-1455.944

PREVIOUS:

CURRENT December 1971

Lithium Tetrafluoroberyllate ( $\text{Li}_2\text{BeF}_4$ ) $\text{Be}_1\text{F}_4\text{Li}_2(\text{cr},\text{l})$

## Beryllium Hydride (BeH)

## IDEAL GAS

$$S^o(298.15 \text{ K}) = 176.822 \text{ J-K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^o(0 \text{ K}) = 319 \pm 29 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^o(298.15 \text{ K}) = 321 \pm 29 \text{ kJ}\cdot\text{mol}^{-1}$$

Electronic Levels and Quantum Weight	
State	$\epsilon_i, \text{cm}^{-1}$
$\Sigma^+$	0
$\Sigma^-$	2

$$\omega_e = 2038.6 \text{ cm}^{-1} \quad \omega_\epsilon = 35.5 \text{ cm}^{-1} \quad \sigma = 1$$

$$B_e = 10.308 \text{ cm}^{-1} \quad r_e = 1.3431 \text{ \AA}$$

## Enthalpy of Formation

Gaydon<sup>1</sup> selected a value of  $2.3 \pm 0.3 \text{ eV}$  ( $53 \pm 7 \text{ kcal}\cdot\text{mol}^{-1}$ ) for  $D_0^*$  as being  $2.2 \text{ eV}$  ( $50.7 \text{ kcal}\cdot\text{mol}^{-1}$ ). Gaydon's<sup>1</sup> value was used in this table.

## Heat Capacity and Entropy

Molecular constants were found in Herzberg.<sup>2</sup>

## References

<sup>1</sup>A. G. Gaydon, "Dissociation Energies and Spectra of Diatomic Molecules," 2nd ed., Chapman and Hall Ltd., London, 261 pp. (1953); refer to p. 221.

<sup>2</sup>G. Herzberg, "Molecular Spectra and Molecular Structure I. Spectra of Diatomic Molecules," D. Van Nostrand Co Inc., New York, (1950).

## MALCOLM W. CHASE

		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p = 0.1 \text{ MPa}$	
		$J \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$	$-G^o - H^o(T_r)/RT_r$	$H^o - H^o(T_r)/RT_r$	$\Delta H^*$
$T \text{ K}$	$C_p^*$	$S^*$	$\Delta H^*$	$\Delta G^*$	$\log K_r$
0	0	0	0	0	INFINITE
100	29.128	144.978	-8.648	318.716	318.716
200	29.149	165.173	-5.777	320.047	-162.636
250	29.171	171.680	-2.864	321.036	-78.535
289.15	29.224	176.822	0	321.197	-61.781
300	29.227	177.003	0.054	321.194	290.773
350	29.344	181.516	1.518	321.036	-42.607
400	29.538	185.446	2.990	320.835	-36.620
450	29.809	188.540	4.473	320.561	275.391
500	30.144	192.693	5.972	320.233	-31.957
600	30.932	197.661	182.620	9.025	287.889
700	31.769	202.492	185.122	12.160	-28.247
800	32.570	206.785	187.556	18.849	-22.677
900	33.296	210.667	189.921	24.593	-18.706
1000	33.937	214.467	192.175	31.170	-15.795
1100	34.496	217.470	194.328	37.730	-13.431
1200	34.982	220.93	196.384	44.285	-12.190
1300	35.404	223.310	198.348	50.745	-11.950
1400	35.774	225.947	200.227	56.009	-11.791
1500	36.998	228.427	202.025	59.603	-6.892
1600	36.185	230.766	203.749	43.228	-5.456
1700	36.641	232.980	205.404	46.879	-4.889
1800	36.871	235.079	206.994	50.535	-4.387
1900	37.079	237.080	208.526	54.253	-3.938
2000	37.269	238.987	210.001	57.970	-3.536
2100	37.443	240.899	211.425	61.706	-3.173
2200	37.603	242.555	212.801	65.458	-2.845
2300	37.752	244.230	214.131	69.226	-2.546
2400	37.892	245.839	215.419	73.008	-2.273
2500	38.023	247.389	216.667	76.804	96.795
2600	38.146	248.883	217.878	80.613	-2.022
2700	38.264	250.324	219.053	84.433	-1.792
2800	38.376	251.718	220.193	88.265	-1.562
2900	38.483	252.067	221.305	92.108	-1.344
3000	38.585	254.273	222.386	95.962	-1.120
3100	38.684	256.560	224.464	100.825	-1.000
3200	38.780	258.669	224.464	103.698	-96.925
3300	38.872	259.064	225.464	107.581	-1.517
3400	38.962	259.216	226.440	111.473	-1.521
3500	39.049	260.357	227.393	115.373	-1.580
3600	39.135	261.458	228.324	120.200	-1.504
3700	39.218	262.531	229.234	123.200	-1.489
3800	39.300	263.578	230.124	127.126	-1.459
3900	39.380	264.560	230.995	131.050	-1.438
4000	39.459	265.598	231.848	135.002	-18.206
4100	39.536	266.573	232.683	138.927	-1.444
4200	39.613	267.527	233.501	142.909	-1.423
4300	39.688	268.560	234.403	146.874	-1.392
4400	39.762	269.573	235.960	150.847	-1.362
4500	39.835	270.582	235.862	154.827	-10.730
5100	40.261	275.890	240.210	178.857	-13.964
5200	40.329	276.062	240.592	182.886	-14.634
5300	40.398	276.144	241.563	186.923	-15.389
5400	40.466	277.527	242.223	192.808	-16.170
5500	40.533	278.330	242.873	195.016	-16.170
5000	40.191	274.483	239.317	174.834	-12.719
5700	40.867	279.061	243.512	199.072	-13.319
5800	40.733	280.488	244.142	203.136	-12.519
5900	40.800	281.185	245.374	207.206	-17.762
6000	40.865	281.871	245.977	211.282	-18.094
				21.837	-1.601

CURRENT, March 1963 (1 atm)

bar

PREVIOUS, March 1963 (1 atm)

Be<sub>1</sub>H<sub>1</sub>(g)

## Beryllium Hydride (BeH)



## IDEAL GAS

**Beryllium Hydroxide (BeOH)**

$$\Delta H^\circ(0\text{ K}) = [209.59 \pm 12.6] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(298.15\text{ K}) = -113.7 \pm 37.7 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(298.15\text{ K}) = -114.6 \pm 37.7 \text{ kJ}\cdot\text{mol}^{-1}$$

Electronic Levels and Quantum Weights	
$\epsilon_i$ , cm <sup>-1</sup>	g <sub>i</sub>
0	[2]
[30000]	[4]
'	[1266](1) [606](2) [3650](1)

Point Group: [C<sub>∞</sub>]

Bond Distances: Be-O = [1.38] Å; O-H = [0.96] Å

σ = 1

Bond Angle: Be-O-H = [180]<sup>o</sup>Rotational Constant: B<sub>0</sub> = [1.29312] cm<sup>-1</sup>

## Enthalpy of Formation

The adopted  $\Delta H^\circ(298.15\text{ K}) = -27.4 \pm 10 \text{ kcal mol}^{-1}$ , which corresponds to  $D\delta(\text{Be}-\text{OH}) = 113.9 \pm 10 \text{ kcal}\cdot\text{mol}^{-1}$ , is derived from 3rd law analysis of Knudsen-cell mass-spectrometric studies and Knudsen-cell weight-loss studies of several BeOH(g) producing reactions.<sup>1-3</sup> The earlier Knudsen-cell mass-spectrometric measurement by Hildenbrand *et al.*<sup>1</sup> had indicated a minimum absolute value of  $\Delta H^\circ(\text{BeOH})$ , g, 298.15 K) = -25 ± 10 kcal·mol<sup>-1</sup>.

Source	Reaction	Data Points	T/K	$\Delta_i H^\circ(298.15\text{ K})$ , 3rd law cal·mol <sup>-1</sup>	Drift cal·K <sup>-1</sup> ·mol <sup>-1</sup>	$\Delta_i H^\circ(298.15\text{ K})$ cal·mol <sup>-1</sup>
Inami and Ju <sup>1</sup>	A	3	2422-2485	9.73 ± 0.93	-13.0 ± 2.0	-27.2
	B	3	2422-2485	0.82 ± 0.59	6.2 ± 5.5	-37.3
	C	3	2422-2485	75.56 ± 1.3	-5.3 ± 17	-16.1
	D	3	2422-2485	12.09 ± 1.8	3.6 ± 25	-29.0
Inami and Ju <sup>2</sup>	E	3	2425-2518	22.11 ± 2.1	-21.3 ± 8.6	-27.1
Ko, Greenbaum, and Farber <sup>3</sup>	F	3	2107-2368	10.01 ± 1.40	5.1 ± 1.7	-39.4

Reactions:	A) Be(Og) + OH(g) = BeOH(g) + O(g)	D) Be(Og) + H(g) = BeOH(g) + Be(g)	
	B) Be <sub>2</sub> O(g) + OH(g) = BeOH(g) + BeO(g)	E) BeCl(g) + OH(g) = BeOH(g) + Cl(g)	
	C) BeO(cr, s) + H(g) = BeOH(g)	F) BeO(cr, a) + OH(g) = BeOH(g)	

The average  $\Delta H^\circ(\text{BeOH})$ , g, 298.15 K) from the measurements of Inami and Ju<sup>1,2</sup> is -27.4 kcal·mol<sup>-1</sup>. The  $\Delta H^\circ(\text{Be}-\text{OH})$ , g, 298.15 K) = 115 kcal·mol<sup>-1</sup> from  $\Delta H^\circ(298.15\text{ K})$  of -27.4 kcal·mol<sup>-1</sup> appears more reasonable than a  $\Delta H^\circ(\text{Be}-\text{OH})$ , g, 298.15 K) = 127 kcal·mol<sup>-1</sup> from the  $\Delta H^\circ(298.15\text{ K})$  of -39.4 kcal·mol<sup>-1</sup>, derived from Ko, Greenbaum, and Farber<sup>3</sup> above. This is based on a comparison of the trends in  $D_0^\circ$  values of the alkaline earth monofluorides and monochlorides and in the adopted  $D_0^\circ$  values for the other alkaline earth monohydroxides.<sup>5</sup> The analogy between gaseous monohydroxides and monohalides, particularly the monofluorides, has already been recognized.<sup>6-9</sup> Accordingly,  $\Delta H^\circ(\text{BeOH})$ , g, 298.15 K) = -27.4 ± 10 kcal·mol<sup>-1</sup> is adopted.

## Heat Capacity and Entropy

The molecular configuration is assumed to be linear in accordance with the prediction of Walsh<sup>10</sup> and the evidence that the gaseous alkali metal monohydroxides are linear.<sup>1-3</sup> By analogy with BeF and BeCl<sup>11</sup> the ground state is assumed to be "2<sup>+</sup>" and the first excited state is estimated at 30000 cm<sup>-1</sup>.

The Be-O bond distance is estimated to be slightly larger, 0.02 Å, than the Be-F bond distance<sup>3</sup> after noting the close similarity in bond distance of the alkali metal fluorides and hydroxides. The O-H bond distance is that in water.<sup>5</sup>

The Be-O stretching frequency, 1266 cm<sup>-1</sup>, is estimated to be the same as the Be-F stretching frequency.<sup>9</sup> The O-H stretching frequency, 3650 cm<sup>-1</sup>, is estimated from the alkali metal hydroxides series. The bending frequency, 606 cm<sup>-1</sup>, is estimated by assuming that the ratio of the bending force constant to the stretching force constant is 0.022, which is the average ratio found in the alkali metal monohydroxides by Acuña and Abramowitz.<sup>9,11</sup>

Continued on page 428

**Be<sub>2</sub>H<sub>2</sub>O<sub>2</sub>(g)****Beryllium Hydroxide (BeOH)**

		Beryllium Hydroxide (BeOH)			Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$		
		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$	$H^\circ - H^\circ(T_r)$	$\Delta_i H^\circ$	$\Delta_i G^\circ$	$\log K_r$	
		$T/K$	$C_p^\circ$	$S^\circ - (G^\circ - H^\circ(T_r))T$	$H^\circ - H^\circ(T_r)$	$\Delta_i H^\circ$	
	0	0	0	INFINITE	-9.558	-113.662	INFINITE
	100	29.307	174.021	240.225	-6.620	-113.745	61.321
	200	33.323	192.328	212.944	-3.523	-114.028	31.594
	250	35.983	203.052	210.212	-1.790	-114.314	25.631
	298.15	38.321	209.594	209.594	0	-114.642	21.769
	300	38.405	209.831	209.595	0.071	-114.655	21.645
	350	40.511	215.914	210.070	2.045	-125.895	18.789
	400	42.314	221.444	211.152	4.117	-115.390	16.640
	450	43.849	226.519	212.581	6.277	-128.905	14.963
	500	45.157	231.208	214.212	8.498	-116.102	13.617
	600	47.250	239.636	217.763	13.123	-116.788	11.590
	700	48.862	247.045	221.428	17.932	-135.803	10.134
	800	50.175	253.658	225.051	22.886	-118.155	9.035
	900	51.295	259.634	228.566	27.961	-118.862	8.175
	1000	52.281	265.090	231.950	33.140	-119.598	7.483
	1100	53.162	270.115	235.194	38.413	-120.371	6.943
	1200	53.936	274.776	238.301	43.770	-121.186	6.436
	1300	54.672	279.123	241.276	49.202	-122.051	6.029
	1400	55.319	283.199	244.126	54.722	-122.972	5.677
	1500	55.901	287.036	246.860	60.264	-123.955	5.270
	1600	56.426	290.661	249.485	65.388	-139.543	5.082
	1700	56.898	294.096	252.009	71.547	-140.267	4.813
	1800	57.324	297.360	254.439	77.259	-141.000	4.573
	1900	57.708	300.470	256.780	83.011	-141.746	4.357
	2000	58.053	303.439	259.040	88.799	-142.550	4.162
	2100	58.366	306.279	261.222	94.620	-143.285	3.984
	2200	58.648	309.001	263.332	100.173	-144.083	3.822
	2300	59.164	311.614	265.375	106.349	-145.903	3.673
	2400	59.156	314.126	267.355	112.251	-145.747	3.535
	2500	59.347	316.544	269.274	118.175	-146.615	3.408
	2600	59.540	318.876	271.137	124.120	-147.509	3.290
	2700	59.715	321.216	272.947	130.083	-148.430	3.180
	2800	59.876	323.201	274.356	136.938	-149.336	2.961
	2900	60.024	325.404	276.419	142.038	-148.655	2.678
	3000	60.139	327.442	278.086	140.174	-149.174	2.413
	3100	60.284	329.416	279.108	154.089	-140.114	2.166
	3200	60.400	331.332	281.294	160.123	-140.069	1.934
	3300	60.507	333.192	282.838	166.169	-140.042	1.717
	3400	60.606	335.000	284.346	172.224	-140.034	1.512
	3500	60.707	336.758	285.818	178.299	-140.047	1.319
	3600	60.787	338.470	287.257	184.364	-140.083	1.136
	3700	60.869	340.136	288.664	190.447	-140.145	0.964
	3800	60.947	341.760	290.040	196.538	-140.235	0.800
	3900	61.021	343.345	291.387	202.636	-140.354	0.645
	4000	61.092	344.890	292.705	208.742	-140.505	0.497
	4100	61.160	346.380	293.962	214.895	-140.690	0.357
	4200	61.226	347.874	295.662	220.974	-140.911	0.223
	4300	61.290	349.316	296.502	227.104	-141.170	0.096
	4400	61.353	350.726	297.718	233.232	-141.470	-0.026
	4500	61.415	352.105	298.912	239.370	-141.811	-0.279
	4600	61.476	353.456	300.083	245.515	-142.197	-0.254
	4700	61.538	354.778	301.332	251.662	-142.628	-0.361
	4800	61.598	361.015	302.362	257.873	-143.107	-0.463
	5000	61.660	367.345	303.471	263.985	-143.655	-0.562
	5000	61.721	358.592	304.561	270.154	-144.212	-0.657
	5100	61.784	369.814	305.632	276.339	-144.842	-0.748
	5200	61.847	376.047	306.686	282.511	-145.524	-0.835
	5300	61.911	362.194	307.722	288.699	-146.259	-0.920
	5300	61.977	363.251	308.741	294.893	-147.084	-1.081
	5300	62.043	364.489	309.445	301.094	-147.852	-1.080
	5600	62.111	365.608	310.732	307.302	-148.791	-1.156
	5700	62.181	366.708	311.705	313.517	-149.746	-1.230
	5800	62.252	367.790	312.662	319.738	-150.756	-1.301
	5900	62.324	368.854	313.606	325.967	-151.703	-1.370
	6000	62.399	369.903	314.535	332.203	-152.943	-1.436

CURRENT December 1975 (1 atm)

PREVIOUS: December 1975 (1 atm)

**Beryllium Hydroxide (BeOH)**

CURRENT December 1975 (1 bar)

Beryllium Hydroxide, Ion (BeOH<sup>+</sup>)

## IDEAL GAS

 $M_r = 26.018971$  Beryllium Hydroxide, Ion (BeOH<sup>+</sup>)

$$S^\circ(298.15 \text{ K}) = [203.9 \pm 6.3] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = 754.70 \pm 50 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(0 \text{ K}) = 754.70 \pm 50 \text{ kJ}\cdot\text{mol}^{-1}$$

Vibrational Frequencies and Degeneracies v, cm <sup>-1</sup>	
[1260] (1)	0
[600] (2)	0.29, 321
[3650] (1)	0.33, 428
	0.36, 103
	0.38, 441
	0.39, 919
	0.39, 157
	0.40, 625
	0.42, 420
	0.43, 946
	0.50, 245
	0.60, 323
	0.70, 592
	0.80, 224
	0.90, 336
	1.00, 316
	1.10, 192
	1.20, 982
	1.30, 695
	1.40, 5338
	1.50, 918
	1.60, 441
	1.70, 5912
	1.80, 336
	1.90, 719
	2.00, 863
	2.10, 375
	2.20, 657
	2.30, 912
	2.40, 143
	2.50, 354
	2.60, 556
	2.70, 721
	2.80, 881
	2.90, 027
	3.00, 162
	3.10, 880
	3.20, 285
	3.30, 399
	3.40, 602
	3.50, 692
	3.60, 775
	3.70, 853
	3.80, 925
	3.90, 992
	4.00, 6055
	4.100, 1113
	4.200, 1168
	4.300, 1220
	4.400, 1268
	4.500, 1313
	4.600, 1355
	4.800, 1433
	4.900, 1469
	5.000, 1502
	5.100, 1693
	5.200, 1564
	5.300, 1593
	5.400, 1620
	5.500, 1645
	5.600, 1670
	5.700, 1693
	5.800, 1715
	5.900, 1735
	6.000, 1755

**Enthalpy of Formation**  
Using mass spectrometric techniques, Inami and Ju<sup>1</sup> determined the appearance potential of BeOH(g) to be  $9.0 \pm 0.5$  eV ( $207.55 \pm 11.53$  kcal·mol<sup>-1</sup>). In the same study, Porter<sup>2</sup> was reported to have said that the appearance potential of a metal hydroxide is expected to be about the same as the corresponding fluoride. In this case, the appearance potential of BeF<sub>2</sub>(g) is  $9.1 \text{ eV}^1$ , which is within  $0.1 \text{ eV}$  of the value for BeOH(g). It is also interesting to note that the ionization potential of Be(g) is  $9.22 \text{ eV}$ . We adopt the experimentally determined appearance potential of  $9.0 \pm 0.5 \text{ eV}$  which refers to the process BeOH(g) + c<sup>-</sup> → BeOH<sup>+(g)</sup> + 2e<sup>-</sup>. Using auxiliary data,<sup>3</sup> we calculate  $\Delta_f H^\circ(0 \text{ K}) = 180.39 \pm 12.0 \text{ kcal}\cdot\text{mol}^{-1}$ . This leads to  $\Delta_f H^\circ(298.15 \text{ K}) = 181.63 \pm 12.0 \text{ kcal}\cdot\text{mol}^{-1}$  for BeOH<sup>+(g)</sup>. The ground state quantum weight is assumed to be the same as that of LiOH(g).<sup>4</sup>

## Heat Capacity and Entropy

The molecular configuration is assumed to be linear since experimental evidence indicates that the gaseous alkali metal hydroxides are linear.<sup>4,5,6</sup> In addition, Walsh<sup>7</sup> had predicted that BAH molecules (H=hydrogen atom) with ten or less valence electrons (BeOH<sup>+</sup> has 8 valence electrons) will be linear in their ground state. The molecule BeOH<sup>+</sup> is isoelectronic with LiOH.<sup>8</sup>

The bond dissociation energy for BeOH<sup>+(g)</sup> = Be<sup>+(g)</sup> + OH<sup>(g)</sup> is fairly close to that for BeOH(13.9 kcal·mol<sup>-1</sup>).<sup>9</sup> This suggests a similar bonding in these two molecules. Thus, bond distances are assumed to be the same as those adopted for BeOH(g).<sup>10</sup> The vibrational frequencies are assumed to be similar to those adopted for BeOH(g).<sup>11</sup> The ground state quantum weight is assumed to be the same as that of LiOH(g).<sup>10</sup>

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- R. F. Porter, personal communication, as referenced by Inami and Ju.<sup>1</sup>
- JANAF Thermochemical Tables; e<sup>-(ref.)</sup>, 3-31-65; Be<sup>+(g)</sup>, 6-30-65; LiOH(g), 6-30-71; BeOH(g), 12-31-75.
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- R. F. Porter, personal communication, as referenced by Inami and Ju.<sup>1</sup>
- JANAF Thermochemical Tables; e<sup>-(ref.)</sup>, 3-31-65; Be<sup>+(g)</sup>, 6-30-65; LiOH(g), 6-30-71; BeOH(g), 12-31-75.
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- A. D. Walsh, J. Chem. Soc. 1953, 2288.

Be<sub>1</sub>H<sub>1</sub>O<sub>1</sub>(g) $M_r = 26.018971$  Beryllium Hydroxide, Ion (BeOH<sup>+</sup>)

$T/K$	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$	
		$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\text{S}^\circ - [\text{G}^\circ - \text{H}^\circ(T_r)/T]$	$\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_f G^\circ$
100	0	0.0	INFINITE	-9.546	754.698
200	29.321	168.260	-234.642	-6.638	-3.535
250	33.428	189.606	207.295	-1.796	-
298.15	36.103	197.356	204.539	0.	-
300	38.441	203.919	203.919	759.934	745.758
350	40.625	210.257	204.397	2.051	745.570
400	42.420	215.803	205.481	1.229	740.703
450	43.946	220.889	206.914	6.289	738.085
500	45.245	225.589	208.550	8.519	762.690
600	47.323	234.031	212.109	13.153	764.091
700	48.922	241.430	215.782	17.988	765.497
800	50.224	248.071	219.411	22.927	768.894
900	51.336	254.052	222.933	28.007	768.269
1000	52.316	259.512	226.322	33.190	769.615
1100	53.192	264.540	229.571	38.466	770.925
1200	53.982	269.203	232.682	43.826	772.191
1300	54.695	273.533	235.660	49.260	783.407
1400	55.338	277.630	238.514	54.762	774.567
1500	55.918	281.468	241.251	60.326	775.664
1600	56.441	285.694	243.879	65.944	762.156
1700	56.912	288.530	246.405	71.612	653.512
1800	57.336	291.795	248.837	77.325	764.839
1900	57.719	294.906	251.180	83.078	766.193
2000	58.063	297.875	253.441	88.688	767.512
2100	58.375	300.716	257.625	94.690	768.813
2200	58.657	303.438	257.737	100.542	767.897
2300	58.912	306.031	259.781	106.420	771.354
2400	59.143	308.563	261.762	112.323	772.590
2500	59.354	310.982	263.683	118.248	773.801
2600	59.546	313.314	265.547	124.193	774.986
2700	59.721	315.364	267.338	130.157	776.144
2800	59.881	317.199	269.119	136.137	779.417
2900	60.027	319.843	270.832	142.132	788.483
3000	60.162	321.880	272.500	148.142	790.637
3100	60.285	323.835	274.125	154.164	792.766
3200	60.399	325.771	275.709	160.199	793.271
3300	60.505	327.631	277.254	166.244	797.005
3400	60.602	329.439	278.763	172.299	800.992
3500	60.692	331.197	280.236	178.364	801.157
3600	60.775	332.908	281.675	184.438	803.029
3700	60.853	334.574	283.082	190.519	805.213
3800	60.925	336.198	284.459	196.608	807.200
3900	60.992	337.781	285.806	202.704	809.157
4000	61.055	339.326	287.125	208.806	811.081
4100	61.113	340.835	288.416	214.915	814.229
4200	61.168	342.308	289.682	221.029	814.823
4300	61.220	343.748	290.923	227.148	816.636
4400	61.268	345.156	292.139	233.273	818.407
4500	61.313	346.533	293.333	239.402	820.135
4600	61.355	347.881	294.504	245.535	821.817
4800	61.433	349.201	295.634	251.673	823.451
4900	61.469	350.494	296.783	257.814	825.035
5000	61.502	353.003	298.982	263.959	826.569
5100	61.534	354.222	300.033	270.226	829.475
5200	61.564	355.417	301.106	282.415	830.845
5300	61.593	356.590	302.142	308.515	832.158
5400	61.620	357.741	303.161	329.733	833.414
5500	61.645	358.872	304.164	303.896	834.611
5600	61.670	359.983	305.151	307.062	835.748
5700	61.693	361.075	306.122	313.230	836.826
5800	61.715	362.148	307.079	319.401	837.843
5900	61.735	363.203	308.021	325.071	838.809
6000	61.755	364.241	308.930	331.748	839.695

PREVIOUS December 1975 (1 atm)

CURRENT December 1975 (1 bar)

Beryllium Hydroxide, Ion (BeOH<sup>+</sup>)

## IDEAL GAS

Beryllium Hydride (BeH<sub>2</sub>)

$$S^{\circ}(298.15 \text{ K}) = [173.1] \text{ J K}^{-1} \text{ mol}^{-1}$$

$$\Delta_f H^{\circ}(\text{K}) = [127.2] \text{ kJ mol}^{-1}$$

$$\Delta_f H^{\circ}(298.15 \text{ K}) = [125.52] \text{ kJ mol}^{-1}$$

## Vibrational Frequencies and Multiplicities

$\nu, \text{cm}^{-1}$	$\sigma = 2$
[2200] (1)	
[1500] (2)	
[1300] (1)	

Ground State Quantum Weight: 1

Point Group: [D<sub>3h</sub>]

Bond Distance: Be-H = [1.34] Å

Bond Angle: H-Be-H = [180]°

Rotational constant: B<sub>0</sub> = [4.657172] cm<sup>-1</sup>

**Enthalpy of Formation**  
Estimated by O'Brien, Perrin and Perrine.<sup>1</sup>

## Heat Capacity and Entropy

Molecular and spectroscopic parameters estimated.

## References

- <sup>1</sup>C. J. O'Brien and J. R. Perrin, Marquardt Corp., Van Nuys, Calif. and J. Perrine, Olin Mathieson Chemical Corp., New York 22, N. Y., Estimation of the Heats of Formation of Gaseous Combustion Product Molecules, (October, 1959).

M<sub>f</sub> = 11.02806 Beryllium Hydride (BeH<sub>2</sub>)Be<sub>2</sub>H<sub>2</sub>(g)

$T/K$	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^{\circ} = 0.1 \text{ MPa}$	
		$S^{\circ} - (G^{\circ} - H^{\circ}(T_r))/T$	$H^{\circ} - H^{\circ}(T_r)/T$	$\Delta_f H^{\circ}$	$\Delta_f G^{\circ}$
0	0	0	-8.714	127.206	INFINITE
100	29.101	141.109	-5.822	127.059	123.071
200	29.204	161.292	-2.910	126.700	119.159
250	29.388	167.843	-1.442	126.180	117.339
298.15	30.370	173.115	0	125.520	115.682
300	30.408	173.303	0.056	125.492	115.622
350	31.659	178.079	13.608	124.715	114.037
400	33.233	182.421	17.338	123.916	112.566
450	34.999	186.421	17.460	123.134	111.195
500	36.842	190.204	17.640	122.397	109.908
600	40.446	197.244	179.585	121.062	107.540
700	43.678	203.727	182.577	105.955	102.362
800	46.434	209.744	185.601	119.943	107.577
900	48.733	215.351	188.599	124.805	110.458
1000	50.634	220.587	191.539	129.048	117.482
1100	52.204	225.489	194.405	134.192	121.816
1200	53.505	230.088	197.189	139.480	126.167
1300	54.389	234.415	199.887	144.836	135.508
1400	55.996	238.495	202.501	150.392	140.554
1500	56.262	242.351	205.030	155.981	144.817
1600	56.912	246.003	207.478	161.640	158.740
1700	57.467	249.470	209.847	167.350	162.973
1800	57.944	252.769	212.140	173.131	167.786
1900	58.357	255.913	214.362	178.947	172.287
2000	58.716	258.916	216.515	184.801	182.632
2100	59.030	261.788	218.503	190.688	186.238
2200	59.306	264.541	220.629	196.605	192.227
2300	59.550	267.183	222.596	202.548	197.971
2400	59.766	269.722	224.507	108.514	202.155
2500	59.958	272.165	226.365	114.501	203.928
2600	60.131	274.520	228.172	120.505	93.102
2700	60.285	276.793	229.931	126.526	92.386
2800	60.425	278.988	231.644	132.562	109.220
2900	60.551	281.110	233.313	138.611	119.037
3000	60.665	283.165	234.941	144.672	124.770
3100	60.768	285.156	236.529	150.743	130.567
3200	60.853	287.087	238.079	156.825	136.255
3300	60.930	288.961	239.593	162.916	142.439
3400	61.029	290.782	241.071	169.015	147.906
3500	61.102	292.532	242.517	175.121	156.433
3600	61.169	294.274	243.931	181.235	167.748
3700	61.231	295.931	245.314	187.355	172.519
3800	61.288	297.585	246.669	193.481	177.451
3900	61.341	299.177	247.995	199.612	187.418
4000	61.390	300.731	249.394	205.749	197.421
4100	61.436	302.247	250.567	211.890	202.448
4200	61.478	303.728	251.815	218.036	207.564
4300	61.518	305.175	253.039	224.186	214.674
4400	61.555	306.590	254.240	230.339	220.847
4500	61.590	307.974	255.419	236.497	228.067
5000	61.758	315.693	262.065	273.504	240.472
5200	61.780	316.893	263.108	279.681	246.634
5300	61.802	318.070	264.134	285.850	251.703
5400	61.822	319.225	265.144	292.041	257.844
5500	61.841	320.360	266.137	298.224	262.453
5600	61.859	321.474	267.115	304.409	268.902
5700	61.876	322.559	268.079	310.596	274.074
5800	61.893	323.646	269.028	316.785	278.842
5900	61.908	324.704	270.982	322.975	281.936
6000	61.923	325.744	270.883	329.166	287.834

CURRENT: December 1960 (1 atm) PREVIOUS: December 1960 (1 atm)

Beryllium Hydride (BeH<sub>2</sub>)Be<sub>2</sub>H<sub>2</sub>(g)

Berillium Hydroxide, Alpha ( $\alpha$ -Be(OH) <sub>2</sub> )		CRYSTAL( $\alpha$ )		Berillium Hydroxide, Alpha (Be(OH) <sub>2</sub> )		Be <sub>2</sub> H <sub>2</sub> O <sub>2</sub> (cr)			
$S^{\circ}(298.15 \text{ K}) = [53.6 \pm 8] \text{ J K}^{-1} \cdot \text{mol}^{-1}$	$\Delta H^{\circ}(0 \text{ K}) = \text{Unknown}$	$\Delta H^{\circ}(298.15 \text{ K}) = -902.9 \pm 2.0 \text{ kJ mol}^{-1}$	$\Delta_f H^{\circ}(298.15 \text{ K}) = -902.9 \text{ kJ mol}^{-1}$	$T/K$	$C_p^{\circ}$	$\frac{\text{Enthalpy Reference Temperature} = T = 298.15 \text{ K}}{\text{J K}^{-1} \cdot \text{mol}^{-1}}$	$\frac{\text{Standard State Pressure} = p^* = 0.1 \text{ MPa}}{\text{J K}^{-1} \cdot \text{mol}^{-1}}$		
<b>Enthalpy of Formation</b>									
Bear and Turnbull <sup>1</sup> measured the enthalpy of solution of $\alpha$ -Be(OH) <sub>2</sub> and Be in 22.6% HF(aq) at 21°C. Combining these results, adjusting to 25°C, and correcting for the small HF concentration differences in the two systems, we calculate $\Delta H^{\circ}(298.15 \text{ K}) = -79.16 \text{ kcal mol}^{-1}$ for the reaction $\text{Be(cr)} + 2\text{H}_2\text{O(l)} = \text{Be(OH)}_2(\text{cr}) + \text{H}_2\text{O(g)}$ . Using auxiliary data, <sup>2,3</sup> we derive $\Delta_f H^{\circ}(298.15 \text{ K}) = -215.8 \text{ kcal mol}^{-1}$ for $\alpha$ -Be(OH) <sub>2</sub> . Since this adopted value is calorimetrically determined and based on well characterized samples, we assign an uncertainty of $\pm 0.5 \text{ kcal mol}^{-1}$ .	0	0	$S^{\circ}$	$\frac{-[G^{\circ} - fH^{\circ}(T)]/T}{\text{J K}^{-1} \cdot \text{mol}^{-1}}$	$H^{\circ} - H^{\circ}(T)/T$	$\frac{\Delta_f H^{\circ}}{\text{J K}^{-1} \cdot \text{mol}^{-1}}$			
Parker <sup>4</sup> recently reviewed data pertaining to the enthalpy of formation of the berillium hydroxides. Her analyses were intended to give additional support to the thermochemical values chosen for Be-O(cr). Our interpretation would differ slightly due to the fact that our $\Delta_f H^{\circ}$ value for Be-O(cr) is different (by 0.3 kcal mol <sup>-1</sup> ) at 298.15 K from that adopted by Parker. <sup>4</sup> Discussed in her review were the enthalpy of solution studies by Fricks and Wulhorst <sup>5</sup> [involving BeO and Be(OH) <sub>2</sub> ] and Matignon and Marchal <sup>6,7</sup> [amorphous Be(OH) <sub>2</sub> ] in 30% HF. In addition there is also an earlier study by Mulert <sup>8</sup> involving amorphous Be(OH) <sub>2</sub> in 20% HF. All these studies are in fair agreement with our adopted value for $\Delta_f H^{\circ}(298.15 \text{ K})$ . These latter studies are thought to be less reliable, however, due to incomplete characterization of the berillium compounds.	100	100	$53.555$	$53.555$	0.	$-902.907$	$-815.933$		
				200	65.701	$53.555$	$0.122$	$-902.923$	$-815.934$
				298.15	66.053	$53.556$	$7.626$	$-903.139$	$-786.150$
				300	82.902	$75.434$	$56.369$	$-902.397$	$-756.595$
				400	92.994	$95.086$	$62.183$	$-901.119$	$-728.004$
				500	103.956	$112.633$	$69.157$	$-901.119$	$-699.527$
				700	107.495	$142.430$	$83.881$	$-897.735$	$-670.787$
				800	110.399	$155.262$	$91.110$	$-895.810$	$-642.532$
				900	112.905	$167.327$	$98.121$	$-893.790$	$-614.498$
				1000					

## Berillium Hydroxide, Alpha ( $\alpha$ -Be(OH)<sub>2</sub>)

$$S^{\circ}(298.15 \text{ K}) = [53.6 \pm 8] \text{ J K}^{-1} \cdot \text{mol}^{-1}$$

### Enthalpy of Formation

Bear and Turnbull<sup>1</sup> measured the enthalpy of solution of  $\alpha$ -Be(OH)<sub>2</sub> and Be in 22.6% HF(aq) at 21°C. Combining these results, adjusting to 25°C, and correcting for the small HF concentration differences in the two systems, we calculate  $\Delta H^{\circ}(298.15 \text{ K}) = -79.16 \text{ kcal mol}^{-1}$  for the reaction  $\text{Be(cr)} + 2\text{H}_2\text{O(l)} = \text{Be(OH)}_2(\text{cr}) + \text{H}_2\text{O(g)}$ . Using auxiliary data,<sup>2,3</sup> we derive  $\Delta_f H^{\circ}(298.15 \text{ K}) = -215.8 \text{ kcal mol}^{-1}$  for  $\alpha$ -Be(OH)<sub>2</sub>. Since this adopted value is calorimetrically determined and based on well characterized samples, we assign an uncertainty of  $\pm 0.5 \text{ kcal mol}^{-1}$ .

Parker<sup>4</sup> recently reviewed data pertaining to the enthalpy of formation of the berillium hydroxides. Her analyses were intended to give additional support to the thermochemical values chosen for Be-O(cr). Our interpretation would differ slightly due to the fact that our  $\Delta_f H^{\circ}$  value for Be-O(cr) is different (by 0.3 kcal mol<sup>-1</sup>) at 298.15 K from that adopted by Parker.<sup>4</sup> Discussed in her review were the enthalpy of solution studies by Fricks and Wulhorst<sup>5</sup> [involving BeO and Be(OH)<sub>2</sub>] and Matignon and Marchal<sup>6,7</sup> [amorphous Be(OH)<sub>2</sub>] in 30% HF. In addition there is also an earlier study by Mulert<sup>8</sup> involving amorphous Be(OH)<sub>2</sub> in 20% HF. All these studies are in fair agreement with our adopted value for  $\Delta_f H^{\circ}(298.15 \text{ K})$ . These latter studies are thought to be less reliable, however, due to incomplete characterization of the berillium compounds.

### Heat Capacity and Entropy

The heat capacity is assumed to be identical to that of the  $\beta$ -phase. The entropy difference between the  $\alpha$  and  $\beta$  phases may be obtained from the solubility data of Fricke and Humme.<sup>9</sup> Both crystalline forms of Be(OH)<sub>2</sub> were dissolved in varying concentrations of aqueous NaOH. By relating the quantities dissolved, we calculate  $\Delta_f G^{\circ}(303 \text{ K}) = -0.5 (\pm 0.2) \text{ kcal mol}^{-1}$  for the process  $\alpha\text{-Be(OH)}_2 = \beta\text{-Be(OH)}_2$ . Using auxiliary data,<sup>2</sup> we find  $\Delta_f S^{\circ}(303 \text{ K}) = -0.8 \text{ cal K}^{-1} \cdot \text{mol}^{-1}$ , from which we calculate and adopt  $S^{\circ}(298.15 \text{ K}) = 12.8 \text{ cal K}^{-1} \cdot \text{mol}^{-1}$  for  $\alpha$ -Be(OH)<sub>2</sub>. We assign an uncertainty of  $\pm 2 \text{ cal K}^{-1} \cdot \text{mol}^{-1}$  to reflect the possible error in this calculation of  $\Delta_f S^{\circ}(303 \text{ K})$ .

### Phase Data

The structural information for  $\alpha$ -Be(OH)<sub>2</sub> via x-ray techniques is not complete.<sup>1-9,11</sup> A tetragonal unit cell has been suggested by Guillenma and Lecoq<sup>11</sup> without supporting data. Bear and Turnbull,<sup>1</sup> following this suggestion and using their x-ray data, calculated a crystal density which was consistent with the two experimentally determined values of Fricke and Severini<sup>12</sup> (helium densitometry and a pycnometric method). This lends support to the premise that  $\alpha$ -Be(OH)<sub>2</sub> has a tetragonal unit cell. The alpha phase is metastable.

### Decomposition Data

$T_{\text{dec}}$  is calculated as the temperature at which  $\Delta_f G^{\circ}$  is zero for the reaction  $\text{Be(OH)}_2(\alpha, \text{cr}) = \text{BeO}(\alpha, \text{cr}) + \text{H}_2\text{O(g)}$ .

### References

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<b>M = 43.02686 Berillium Hydroxide, Alpha (Be(OH)<sub>2</sub>)<sub>2</sub></b>		<b>CRYSTAL(<math>\alpha</math>)</b>		<b>Berillium Hydroxide, Alpha (Be(OH)<sub>2</sub>)</b>		<b>Be<sub>2</sub>H<sub>2</sub>O<sub>2</sub>(cr)</b>			
$\Delta H^{\circ}(0 \text{ K}) = \text{Unknown}$	$\Delta_f H^{\circ}(298.15 \text{ K}) = -902.9 \pm 2.0 \text{ kJ mol}^{-1}$	$T/K$	$C_p^{\circ}$	$\frac{\text{Enthalpy Reference Temperature} = T = 298.15 \text{ K}}{\text{J K}^{-1} \cdot \text{mol}^{-1}}$	$\frac{\text{Standard State Pressure} = p^* = 0.1 \text{ MPa}}{\text{J K}^{-1} \cdot \text{mol}^{-1}}$				
<b>Enthalpy of Formation</b>									
Bear and Turnbull <sup>1</sup> measured the enthalpy of solution of $\alpha$ -Be(OH) <sub>2</sub> and Be in 22.6% HF(aq) at 21°C. Combining these results, adjusting to 25°C, and correcting for the small HF concentration differences in the two systems, we calculate $\Delta H^{\circ}(298.15 \text{ K}) = -79.16 \text{ kcal mol}^{-1}$ for the reaction $\text{Be(cr)} + 2\text{H}_2\text{O(l)} = \text{Be(OH)}_2(\text{cr}) + \text{H}_2\text{O(g)}$ . Using auxiliary data, <sup>2,3</sup> we derive $\Delta_f H^{\circ}(298.15 \text{ K}) = -215.8 \text{ kcal mol}^{-1}$ for $\alpha$ -Be(OH) <sub>2</sub> . Since this adopted value is calorimetrically determined and based on well characterized samples, we assign an uncertainty of $\pm 0.5 \text{ kcal mol}^{-1}$ .	0	0	$53.555$	$53.555$	0.	$-902.907$	$-815.933$		
Parker <sup>4</sup> recently reviewed data pertaining to the enthalpy of formation of the berillium hydroxides. Her analyses were intended to give additional support to the thermochemical values chosen for Be-O(cr). Our interpretation would differ slightly due to the fact that our $\Delta_f H^{\circ}$ value for Be-O(cr) is different (by 0.3 kcal mol <sup>-1</sup> ) at 298.15 K from that adopted by Parker. <sup>4</sup> Discussed in her review were the enthalpy of solution studies by Fricks and Wulhorst <sup>5</sup> [involving BeO and Be(OH) <sub>2</sub> ] and Matignon and Marchal <sup>6,7</sup> [amorphous Be(OH) <sub>2</sub> ] in 30% HF. In addition there is also an earlier study by Mulert <sup>8</sup> involving amorphous Be(OH) <sub>2</sub> in 20% HF. All these studies are in fair agreement with our adopted value for $\Delta_f H^{\circ}(298.15 \text{ K})$ . These latter studies are thought to be less reliable, however, due to incomplete characterization of the berillium compounds.	100	100	$53.555$	$53.555$	0.	$-902.907$	$-815.933$		
				200	65.701	$53.555$	$0.122$	$-902.923$	$-815.934$
				298.15	66.053	$53.556$	$7.626$	$-903.139$	$-786.150$
				300	82.902	$75.434$	$56.369$	$-902.397$	$-756.595$
				400	92.994	$95.086$	$62.183$	$-901.119$	$-728.004$
				500	103.956	$112.633$	$69.157$	$-901.119$	$-699.527$
				700	107.495	$142.430$	$83.881$	$-897.735$	$-670.787$
				800	110.399	$155.262$	$91.110$	$-895.810$	$-642.532$
				900	112.905	$167.327$	$98.121$	$-893.790$	$-614.498$
				1000					

PREVIOUS: December 1966

CURRENT: December 1975

Beryllium Hydroxide, Beta ( $\beta$ -Be(OH)<sub>2</sub>)CRYSTAL( $\beta$ )

$$S^\circ(298.15\text{ K}) = [50.2 \pm 4.2] \text{ J K}^{-1}\text{mol}^{-1}$$

$$T_{d,m} = [366]\text{ K}$$

## Enthalpy of Formation

Bear and Turnbull<sup>1</sup> measured the enthalpy of solution of  $\beta$ -Be(OH)<sub>2</sub> and Be in 22.6% HF(aq) at 21°C. Combining these results, adjusting to 25°C, and correcting for the small HF concentration differences in the two systems, we calculate  $\Delta H^\circ(298.15\text{ K}) = -79.89 \text{ kcal}\cdot\text{mol}^{-1}$  for the reaction  $\text{Be}(\text{cr}) + 2\text{H}_2\text{O}(\text{l}) \rightarrow \text{Be}(\text{OH})_2(\text{p}, \text{cr}) + \text{H}_2\text{O}(\text{g})$ . Using auxiliary data,<sup>2,3</sup> we derive  $\Delta H^\circ(298.15\text{ K}) = -216.5 \text{ kcal}\cdot\text{mol}^{-1}$  for  $\beta$ -Be(OH)<sub>2</sub>. Since this adopted value is calorimetrically determined and based on well characterized samples, we assign an uncertainty of  $\pm 0.5 \text{ kcal}\cdot\text{mol}^{-1}$ .

Parker<sup>4</sup> recently reviewed data pertaining to the enthalpy of formation of the beryllium hydroxides. Her analyses were intended to give

additional support to the thermodynamical values chosen for Be(Ocr). Our interpretation would differ slightly due to the fact that our  $\Delta H^\circ$  value for Be(Ocr) is different (by 0.3 kcal·mol<sup>-1</sup> at 298.15 K) from that adopted by Parker.<sup>4</sup> Discussed in her review were the enthalpy of solution studies by Fricke and Wulffhorst<sup>5</sup> [involving BeO and  $\beta$ -Be(OH)<sub>2</sub>] in 11.59% HF and Matignon and Marchal<sup>6</sup> [amorphous Be(OH)<sub>2</sub>] in 30% HF. In addition there is also an earlier study by Muler<sup>7</sup> involving amorphous Be(OH)<sub>2</sub> in 20% HF. These latter three studies are in fair agreement with our adopted value for  $\Delta H^\circ(298.15\text{ K})$  but are thought to be less reliable, however, due to incomplete characterization of the beryllium compounds.

Fricke and Severin<sup>8</sup> and Baur and Lecocq<sup>9</sup> measured the decomposition pressure of water vapor over  $\beta$ -Be(OH)<sub>2</sub>. Fricke and Severin<sup>8</sup> observed a decomposition temperature at 105°C at a pressure of 100 mm Hg while Baur and Lecocq<sup>9</sup> observed 223°C for the equilibrium with saturated water vapor at 24.2 atm. We reduce the latter data to a standard state value  $\Delta G^\circ(496\text{ K}) = -3028 \text{ cal}\cdot\text{mol}^{-1}$  for the decomposition reaction  $\text{Be}(\text{OH})_2(\text{p}, \text{cr}) \rightarrow \text{BeO}(\text{a}, \text{cr}) + \text{H}_2\text{O}(\text{g})$ . The 3rd law analyses for these two decomposition studies are given below where  $\Delta H^\circ(298.15\text{ K})$  refers to the enthalpy of formation of  $\beta$ -Be(OH)<sub>2</sub>.

Source	T/K	Method	$\text{cal}\cdot\text{mol}^{-1}$		
			$\Delta H^\circ(298.15\text{ K})$	$\Delta fT^\circ(298.15\text{ K})$	$\Delta G^\circ(496\text{ K})$
Fricke and Severin <sup>8</sup>	378	K <sub>p</sub>	15.27	$\geq -218.5$	$\geq -218.1$
Baur and Lecocq <sup>9</sup>	496	K <sub>p</sub>	14.88		

These values are within 2 kcal·mol<sup>-1</sup> of our adopted  $\Delta H^\circ(298.15\text{ K})$  value. The difference may be due to the formation of metastable BeO. Fricke and Severin<sup>8</sup> reported that BeO had a distorted lattice which would suggest a  $\Delta H^\circ$  value more positive than  $-145.4 \text{ kcal}\cdot\text{mol}^{-1}$ . Thus, we conclude that these two studies<sup>8,9</sup> are consistent with our adopted value but are not sufficiently definitive for further consideration.

## Heat Capacity and Entropy

The heat capacity is estimated from that for Mg(OH)<sub>2</sub> by subtracting the values for MgO(cr) and adding those for BeO(cr, cr).<sup>2</sup> The entropy is estimated to be  $S^\circ(298.15\text{ K}) = 12.0 \text{ cal}\cdot\text{K}^{-1}\text{mol}^{-1}$ . This value is a compromise of values suggested by two different paths. Additive entropy constants of Kelley<sup>11</sup> yield  $S^\circ(298.15\text{ K}) = 13.20 \text{ cal}\cdot\text{K}^{-1}\text{mol}^{-1}$  whereas a comparison of entropy differences for the alkali metal and alkaline earth chlorides and hydroxides suggest values in the range 10.2 to 12.4 cal·K<sup>-1</sup>mol<sup>-1</sup>. Our adopted value is the same as that selected by NBS.<sup>12</sup>

## Phase Data

Bear and Turnbull<sup>1</sup> and Seitz *et al.*,<sup>13</sup> using x-ray powder techniques, determined that  $\beta$ -Be(OH)<sub>2</sub> has an orthorhombic structure, the  $\epsilon$ -Zn(OH)<sub>2</sub> structure. The  $\beta$ -structure is the stable crystalline form for Be(OH)<sub>2</sub> whereas the  $\alpha$ -structure is metastable.

## Decomposition Data

$T_{\alpha\text{m}}$  is calculated as the temperature at which  $\Delta G^\circ$  is zero for the reaction  $\text{Be}(\text{OH})_2(\text{p}, \text{cr}) \rightarrow \text{BeO}(\alpha, \text{cr}) + \text{H}_2\text{O}(\text{g})$ .

## References

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PREVIOUS - December 1966

CURRENT December 1975

Beryllium Hydroxide, Beta (Be(OH)<sub>2</sub>)Be<sub>2</sub>H<sub>2</sub>O<sub>2</sub>(cr)

T/K	C <sub>p</sub>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>0</sup> = 0.1 MPa	
		$S^\circ - [G^\circ - f(T)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta H^\circ$	$\Delta G^\circ$
0	0	0	0	0	0
100	50.208	50.208	0	-905.836	-817.864
200	50.615	50.209	0.122	-905.832	-817.318
298.15	51.022	51.022	0.7656	-906.067	-787.740
300	51.022	51.022	16.451	-905.326	-758.230
400	52.902	72.087	63.810	26.086	-728.924
500	52.994	91.739	58.836	36.261	-902.456
600	59.387	109.286	63.161	-699.859	52.224
700	103.956	124.963	80.533	-900.664	-671.038
800	107.495	139.082	57.737	-898.739	-642.149
900	110.399	151.915	68.906	-896.719	-614.080
1000	112.905	163.880			





**Beryllium Iodide ( $\text{BeI}_2$ )****CRYSTAL** **$M_r = 262.82118$  Beryllium Iodide ( $\text{BeI}_2$ )** **$\text{BeI}_2(\text{cr})$** 

$$\Delta H^\circ(298.15 \text{ K}) = [120.5 \pm 4.2] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{fus}} = 753 \pm 15 \text{ K}$$

$$\Delta H^\circ(298.15 \text{ K}) = [-188.7 \pm 21] \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta_{\text{fus}}H^\circ = [20.9 \pm 12.6] \text{ kJ} \cdot \text{mol}^{-1}$$

**Enthalpy of Formation**

A direct measurement of the enthalpy of formation has not been made. An estimate of  $\Delta H^\circ$  is obtained by a method suggested by Parker<sup>1</sup> and used in the  $\text{BeBr}_2(\text{cr})$  table.<sup>2</sup> Blitz and Messerknecht<sup>3</sup> have measured the enthalpies of solution of  $\text{BeCl}_2(\text{cr})$  and  $\text{BeI}_2(\text{cr})$  in aqueous  $\text{HCl}$  (18.69%). Samples<sup>4</sup> of the dihalides were prepared from reactions of  $\text{BeO}-\text{C}$  mixtures with the halogens at elevated temperatures. We assume that the two dihalides had similar structures, i.e. the  $\alpha$ -form (orthorhombic).  $\Delta H^\circ(\text{BeI}_2, 298.15 \text{ K})$  is estimated at  $-109.1 \text{ kcal} \cdot \text{mol}^{-1}$  by combining  $\Delta H^\circ$  of  $\text{BeCl}_2(\text{cr})$  with  $\Delta H^\circ(\text{BeBr}_2, \text{cr}, \alpha, 298.15 \text{ K}) = -117.3 \pm 0.8 \text{ kcal} \cdot \text{mol}^{-1}$ , and twice the difference in  $\Delta H^\circ(\text{HCl}/\text{H}_2\text{O}, 298.15 \text{ K})$  and  $\Delta H^\circ(\text{HBr}/\text{H}_2\text{O}, 298.15 \text{ K})$  which is  $-52.3 \text{ kcal} \cdot \text{mol}^{-1}$ .<sup>5</sup> The enthalpy associated with the aqueous anions is assumed to be negligible. Combination of the estimated value for  $\Delta H^\circ(\text{BeI}_2, 18.8\% \text{ HCl}, 298.15 \text{ K})$  with  $\Delta H^\circ = -62.5 \text{ kcal} \cdot \text{mol}^{-1}$ , gives  $\Delta H^\circ(\text{BeI}_2, \text{cr}, 298.15 \text{ K}) = -46.6 \text{ kcal} \cdot \text{mol}^{-1}$ , which is within 0.6  $\text{kcal} \cdot \text{mol}^{-1}$  of the value suggested by NBS.<sup>6</sup> Subsequent measurements by Blitz *et al.*<sup>7</sup> in less concentrated  $\text{HCl}$  (1.48%) solution leads to  $\Delta H^\circ(298.15 \text{ K}) = -43.6 \text{ kcal} \cdot \text{mol}^{-1}$  by a similar route. We adopt an average value of  $-45.1 \text{ kcal} \cdot \text{mol}^{-1}$  but emphasize that the uncertainty in  $\Delta H^\circ$  is much greater than indicated (3  $\text{kcal} \cdot \text{mol}^{-1}$ ) by the closeness of these two values. An uncertainty of  $\pm 0.5 \text{ kcal} \cdot \text{mol}^{-1}$  is believed to be more realistic.

**Heat Capacity and Entropy**

No low-temperature heat capacity or high-temperature enthalpy measurements have been reported. We estimate  $C_p^\circ(298.15 \text{ K}) = 16.482 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  from the reaction  $\text{BeCl}_2(\text{cr}, \alpha) + 2\text{LiI}(\text{cr}) = \text{BeI}_2(\text{cr}) + 2\text{LiCl}(\text{cr})$  by assuming  $\Delta C_p^\circ = 0$ . Similar results are obtained using  $\text{BeF}_3$  values above 298.15 K are assumed to parallel those for  $\alpha\text{-BeCl}_2$ .

Application of the Berthelot principle<sup>8</sup> to the process  $\text{BeI}_2(\text{cr}) + \text{Be}(\text{cr}) \rightarrow \text{Ba}(\text{cr}) + \text{BeI}_2(\text{cr})$  suggests  $S^\circ(298.15 \text{ K}) = 26.8 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ . A graphical comparison of the standard entropies for other alkaline-earth dihalides<sup>2</sup> indicates that this value is reasonable. Other estimated values are given by additive entropy constants (27.4  $\text{cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ ),<sup>9</sup> Brewer (31.0  $\text{cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ ),<sup>10</sup> and Brewer *et al.* (25  $\text{cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ ).<sup>11</sup> For additional information of the heat capacity and entropy, refer to the enthalpy of formation discussion for gaseous  $\text{BeI}_2$ .

**Fusion Data**

Refer to the liquid table for details.

**Phase Data**

Semenenko and Naumova<sup>12</sup> studied the  $\text{BeI}_2$  crystal modifications by thermal and x-ray techniques. The study was complicated by the extreme hygroscopicity, high vapor pressures near the melting point, and susceptibility to oxidation by traces of oxygen. As stated by Semenenko and Naumova, the sequence of polymorphic conversion and the character of the resulting modifications of  $\text{BeI}_2$ , which are largely dependent on the heating and cooling conditions, parallel those of  $\text{BeCl}_2$ .<sup>13</sup> They detected thermally transitions at 290°C, 370°C, and a melting at 490°C. However, this data does not appear to be fully consistent in terms of crystallographic structures with that proposed by Johnson, Staritzky, and Douglas,<sup>14</sup> and Messerknecht and Blitz.<sup>15</sup> These latter works suggested two structures with a transition at 350°C. We assume the similarity with  $\text{BeCl}_2$  with a transition in the vicinity of 350–370°C. Further study is necessary to resolve all possible phases and their structures.

**Sublimation Data**

Refer to the ideal gas table for details.

**References**

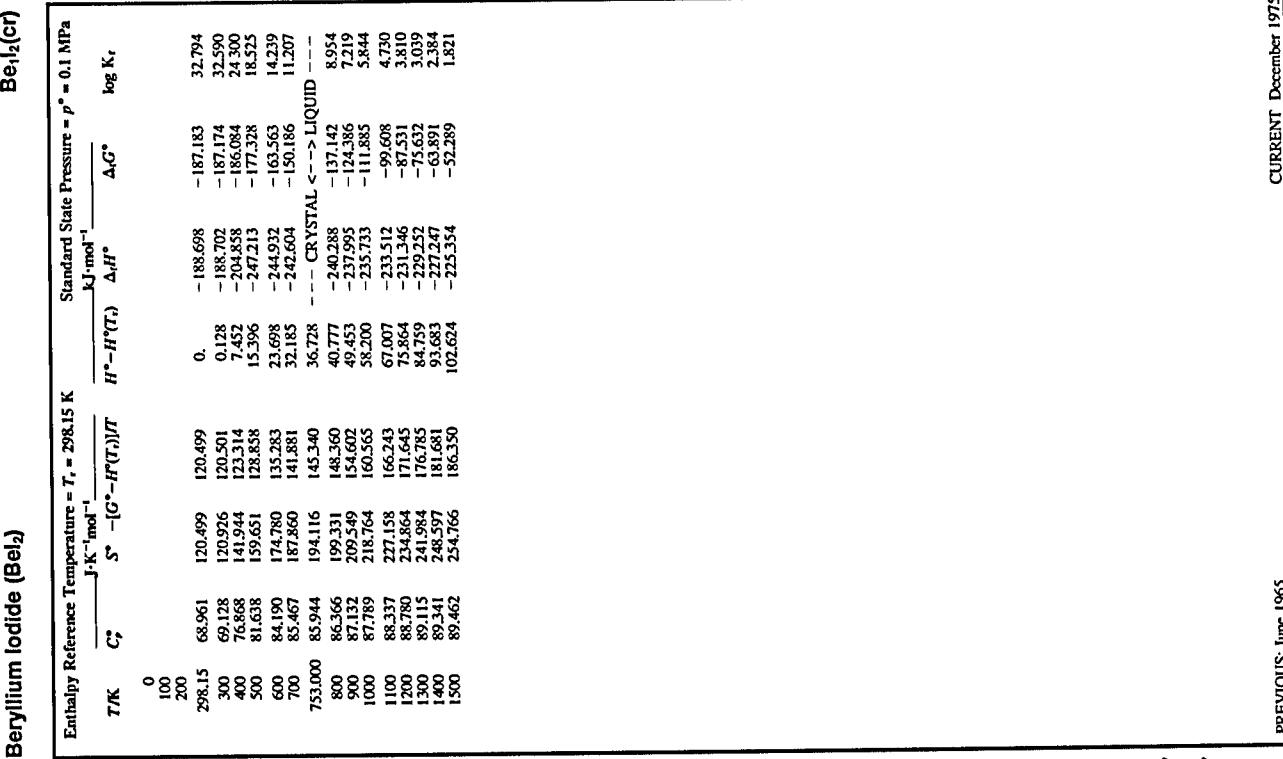
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**Beryllium Iodide ( $\text{BeI}_2$ )**

PREVIOUS: June 1965

CURRENT: December 1975

Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$						Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$			
			$C_p^\circ$	$S^\circ$	$-\left[G^\circ - H^\circ(T_r)\right]/T$	$H^\circ - H^\circ(T_r)/T$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	$\log K_r$
0									
100									
200	298.15	68.961	120.499	120.499	0.	-188.698	-187.183	-187.183	32.794
300	298.15	69.128	120.501	120.501	0.128	-188.702	-187.174	-187.174	32.590
400	298.15	76.868	123.944	123.944	7.452	-204.858	-186.084	-186.084	18.520
500	298.15	81.638	128.858	128.858	15.396	-247.213	-177.328	-177.328	18.255
600	298.15	84.190	124.780	125.283	23.698	-244.932	-163.563	-163.563	14.239
700	298.15	85.467	127.860	141.881	32.185	-242.604	-150.186	-150.186	11.207
753.000	298.15	85.944	145.340	145.340	36.728	— CRYSTAL —	— LIQUID —	— LIQUID —	—
800	298.15	86.366	149.331	148.360	40.777	-240.288	-137.142	-137.142	8.954
900	298.15	87.132	154.602	154.602	49.453	-257.995	-124.386	-124.386	7.219
1000	298.15	87.789	160.565	160.565	58.200	-255.733	-111.885	-111.885	5.844
1100	298.15	88.337	166.243	166.243	67.007	-233.512	-99.508	-99.508	4.730
1200	298.15	88.780	171.645	171.645	75.864	-231.346	-87.531	-87.531	3.810
1300	298.15	89.115	176.735	176.735	84.759	-229.252	-75.632	-75.632	3.019
1400	298.15	89.341	181.881	181.881	93.853	-227.247	-63.391	-63.391	2.384
1500	298.15	89.462	186.330	186.330	102.624	-225.354	-52.289	-52.289	1.821



Beryllium Iodide ( $\text{BeI}_2$ )

## LIQUID

$$\begin{aligned} S^\circ(298.15 \text{ K}) &= [128.999] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1} \\ T_{\text{fus}} &= 753 \pm 15 \text{ K} \end{aligned}$$

**Enthalpy of Formation**

The enthalpy of formation is calculated from that of the crystal by adding  $\Delta_{\text{fus}}H^\circ$  and the difference enthalpy,  $H^\circ(753 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and liquid.

**Heat Capacity and Entropy**

The heat capacity is estimated by comparison with the measured value for  $\text{BeCl}_2$ .<sup>1</sup> A glass transition is assumed at 400 K below which the heat capacity is that of the crystal. The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

**Fusion Data**

Rahlf and Fischer<sup>2</sup> reported a melting point of 753 K. Semeneko and Naumova,<sup>3</sup> using thermal analysis techniques, implied a melting point of 763 K. Since this latter value was derived from a thermogram, it is probable that this value represents a maximum, with the true melting point somewhat lower. We adopt  $T_{\text{fus}} = 753 \pm 15 \text{ K}$ . We estimate the enthalpy of melting,  $\Delta_{\text{fus}}H^\circ = 5.0 \pm 3.0 \text{ kcal}\cdot\text{mol}^{-1}$ . This estimate includes a contribution for melting (based on the entropy of melting for other alkaline earth dihalides) and a contribution for a phase transition. There is no experimental data available pertaining to the enthalpy of melting.

**Vaporization Data**

$T_{\text{vap}}$  is the temperature at which  $\Delta_G^\circ = 0$  for the process  $\text{BeI}_2(\text{l}) = \text{BeI}_2(\text{g})$ .  $\Delta_{\text{vap}}H^\circ$  is the corresponding difference in the  $\Delta_H^\circ$  values for the liquid and gas at  $T_{\text{vap}}$ .

**References**

<sup>1</sup>JANAF Thermochemical Table:  $\text{BeCl}_2(\text{l})$ , 6-30-65.

<sup>2</sup>O. Rahlf and W. Fischer, Z. Anorg. Chem. 211, 349 (1933).

<sup>3</sup>K. N. Semeneko and J. N. Naumova, Russ. J. Structural Chem. 4, 59 (1963).

 **$M_r = 262.82118$  Beryllium Iodide ( $\text{BeI}_2$ )**

$T/\text{K}$	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$	
		$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$-[G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_H^\circ$
0					
100					
200	68.961	128.999	128.999	0.	-178.377
298.15	68.961	128.999	128.999	0.	-178.396
300	69.128	129.426	129.000	0.128	-178.380
400	76.988	150.434	131.812	7.449	-194.539
400,000	76.988	150.434	131.812	7.449	GLASS $\leftarrow \rightarrow$ LIQUID
400,000	112.968	150.434	131.812	7.449	TRANSITION
500	112.968	175.643	138.151	171.653	17.932
600	112.968	196.239	146.168	159.773	13.909
700	112.968	213.653	154.597	223.128	11.101
753,000	112.968	22.198	159.047	47.327	CRYSTAL $\leftarrow \rightarrow$ LIQUID
800	112.968	228.738	162.943	52.636	138.386
900	112.968	242.044	171.007	63.933	128.330
1000	112.968	253.946	178.716	75.230	119.715
1100	112.968	264.713	186.053	86.527	111.077
1200	112.968	274.542	193.023	97.823	102.863
1300	112.968	283.385	199.646	109.120	93.030
1400	112.968	291.957	205.944	120.417	87.538
1500	112.968	299.751	211.941	131.714	80.355

$T/\text{K}$	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$	
		$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$-[G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_H^\circ$
0					
100					
200	68.961	128.999	128.999	0.	-178.377
298.15	68.961	128.999	128.999	0.	-178.396
300	69.128	129.426	129.000	0.128	-179.402
400	76.988	150.434	131.812	7.449	-179.162
400,000	76.988	150.434	131.812	7.449	31.396
400,000	112.968	150.434	131.812	7.449	log $K_r$
500	112.968	175.643	138.151	187.449	
600	112.968	196.239	146.168	208.746	
700	112.968	213.653	154.597	228.266	
753,000	112.968	22.198	159.047	233.542	
800	112.968	228.738	162.943	242.044	
900	112.968	242.044	171.007	253.946	
1000	112.968	253.946	178.716	264.713	
1100	112.968	264.713	186.053	274.542	
1200	112.968	274.542	193.023	283.385	
1300	112.968	283.385	199.646	291.957	
1400	112.968	291.957	205.944	299.751	
1500	112.968	299.751	211.941	31.714	

**Beryllium Iodide ( $\text{BeI}_2$ )**  
PREVIOUS: June 1965  
CURRENT December 1975

## CRYSTAL-LIQUID

***M<sub>r</sub>* = 262.82118 Beryllium Iodide (BeI<sub>2</sub>)**

0 to 753 K  
above 753 K

crystal

liquid

Refer to the individual tables for details.

T/K	C <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K			Standard State Pressure = p <sup>o</sup> = 0.1 MPa			
		J/K <sup>-1</sup> mol <sup>-1</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )/T	kJ/mol <sup>-1</sup>	ΔH <sup>o</sup>	kJ/mol <sup>-1</sup>	log K <sub>r</sub>
0								
100								
200	298.15	68.961	120.499	120.499	0.	-188.698	-187.183	32.794
300	69.128	120.976	120.501	0.128	-188.702	-187.174	32.580	
400	76.868	141.944	123.314	7.452	-204.838	-186.084	24.300	
500	81.638	159.651	128.838	15.396	-247.213	-177.328	18.525	
600	84.190	174.780	135.283	23.698	-244.932	-163.563	14.239	
700	85.467	187.860	141.1881	32.185	-242.604	-150.186	11.207	
753.000	85.944	194.116	145.340	36.728	—	—	—	
753.000	112.968	221.898	145.340	57.648	CRYSTAL <--> LIQUID TRANSITION	CRYSTAL <--> LIQUID TRANSITION	CRYSTAL <--> LIQUID TRANSITION	
800	112.968	228.738	150.041	62.958	-218.107	-138.486	9.042	
900	112.968	242.044	159.539	74.254	-213.193	-128.830	7.477	
1000	112.968	253.946	168.395	85.551	-208.381	-119.715	6.253	
1100	112.968	264.713	176.669	96.848	-203.671	-111.077	5.275	
1200	112.968	274.542	184.422	108.145	-199.065	-102.863	4.478	
1300	112.968	283.585	191.707	119.442	-194.569	-95.030	3.818	
1400	112.968	291.957	198.572	130.738	-190.192	-87.538	3.266	
1500	112.968	299.751	205.060	142.035	-185.943	-80.354	2.798	

PREVIOUS

CURRENT December 1975

Beryllium Iodide (BeI<sub>2</sub>)

**Beryllium Iodide (BeI<sub>2</sub>)****IDEAL GAS****Beryllium Iodide (BeI<sub>2</sub>)**

$$\Delta_f H^\circ(0\text{ K}) = -62.5 \pm 33.5 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15\text{ K}) = [291.52 \pm 2.1] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_a H^\circ(0\text{ K}) = -62.5 \pm 33.5 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_a H^\circ(298.15\text{ K}) = -64.0 \pm 33.5 \text{ kJ}\cdot\text{mol}^{-1}$$

**Vibrational Frequencies and Degeneracies**

$$v, \text{ cm}^{-1}$$

Ground State Quantum Weight: [1]  
Point Group: D<sub>ab</sub>  
Bond Distance: Be-I = 2.12 ± 0.05 Å  
Bond Angle: I-Be-I = 180° ± 10°  
Rotational Constant: B<sub>0</sub> = 0.014778 cm<sup>-1</sup>

**Enthalpy of Formation**

Rahlf's and Fischer<sup>1</sup> have reported measurements of the sublimation pressures (578–703 K, 9 pis) for BeI<sub>2</sub>. The measurements were complicated by reaction of the diiodide with the quartz apparatus. Assuming the reaction to be BeI<sub>2</sub>(cr) + SiO<sub>2</sub>(cr) = SiI<sub>4</sub>(g) + 2BeO(cr), Rahlf's and Fischer<sup>1</sup> corrected their measured total pressure for the partial pressure of the tetraiodide. A 2nd and 3rd law analysis of their corrected data yields Δ<sub>ad</sub>H<sup>°</sup>(298.15 K) = 29.8 ± 0.29 kcal·mol<sup>-1</sup> (3rd law) and 28.34 ± 0.74 kcal·mol<sup>-1</sup> (2nd law) with a drift of 2.2 ± 1.3 cal·K<sup>-1</sup>·mol<sup>-1</sup>. We adopt Δ<sub>ad</sub>H<sup>°</sup>(298.15 K) = 15.3 kcal·mol<sup>-1</sup>. We have assumed negligible dimer formation Δ<sub>dH</sub>(298.15 K) = -15.3 kcal·mol<sup>-1</sup> for BeI<sub>2</sub>(cr) when the adopted Δ<sub>ad</sub>H<sup>°</sup>(298.15 K) value is added to the Δ<sub>dH</sub>(298.15 K) value for BeI<sub>2</sub>(cr).

The drift could be reduced by further adjusting the Gibbs energy functions for the crystal. These functions may be changed by altering the C<sub>p</sub> values and/or the S<sup>°</sup>(298.15 K) value. Such changes would yield values which are unreasonable when compared to other alkaline earth dihalides. Note also that a similar sublimation study for BaCl<sub>2</sub><sup>2</sup> gives a drift of -1.3 ± 2.6 cal·K<sup>-1</sup>·mol<sup>-1</sup>. We tentatively assume the drift is due to the data rather than our choice of functions.

**Heat Capacity and Entropy**

Electron diffraction patterns for BeI<sub>2</sub> vapor<sup>4</sup> have been interpreted in terms of a linear configuration, with the latter study reporting the Be-I bond distance as 2.12 Å. Other studies also suggest a linear molecule. For example, the electric deflection of mass spectrometrically detected molecular beams<sup>5</sup> showed that all the beryllium dihalides are linear.

Snelson<sup>6</sup> observed the infrared spectrum of BeI<sub>2</sub> in the spectral range 4000–200 cm<sup>-1</sup> using a matrix isolation technique. Assuming a linear geometry, v<sub>3</sub> was assigned as 873 cm<sup>-1</sup>. Snelson<sup>6</sup> estimated a value for v<sub>2</sub> based on force constant values for the other three beryllium dihalides. The values of v<sub>1</sub> were calculated using a simple valence force field approximation. We adopt the two estimated and one measured vibrational frequency as reported by Snelson.<sup>6</sup> The ground state quantum weight of one is assigned by analogy with BaCl<sub>2</sub><sup>2</sup>.

Brewer et al.<sup>7</sup> have tabulated Gibbs energy functions for BeI<sub>2</sub> up to 2000 K. Their values are consistently lower than ours due primarily to their use of a higher bending frequency (v<sub>2</sub> = 395 cm<sup>-1</sup>).

**References**

- O. Rahlf's and W. Fischer, Z. Anorg. Chem. 211, 349 (1933).
- JANAF Thermochemical Tables, BeCl<sub>2</sub>(O), 6–30–65.
- P. S. Aikhin and V. P. Spiridonov, Kristallografiya 2, 472 (1957).
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- A. Buchler, J. L. Stauffer, and W. Klemperer, J. Amer. Chem. Soc. 86, 4544 (1964).
- A. Snelson, J. Phys. Chem. 72, 250 (1968).
- L. Brewer, G. R. Somoyajulu, and E. Brackett, Chem. Revs. 63, 111 (1963).

CURRENT December 1975 (1 bar)

PREVIOUS December 1975 (1 atm)

Beryllium Iodide (BeI <sub>2</sub> )									
M <sub>r</sub> = 262.82118      Beryllium Iodide (BeI <sub>2</sub> )									
Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K      Standard State Pressure = p <sup>°</sup> = 0.1 MPa									
T/K	C <sub>p</sub> <sup>°</sup>	S <sup>°</sup>	-G <sup>°</sup> -RT(T <sub>r</sub> )/RT	H <sup>°</sup> -H <sup>°</sup> (T <sub>r</sub> )	kJ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	ΔG <sup>°</sup>
0	0	0	INFINITE	-13.633	-62.517	-62.517	-62.517	-62.517	INFINITE
100	44.605	236.565	337.992	-10.143	-62.117	-79.624	-41.591	-41.591	
200	51.767	270.220	296.456	-2.247	-62.731	-96.949	25.320	22.030	
250	53.542	281.970	292.421	-2.613	-63.316	-105.439	14.330		
298.15	54.939	291.524	291.524	0.	-64.015	-113.491	19.883		
300	56.181	300.433	292.199	2.882	-64.935	-122.021	18.211		
350	57.156	308.001	293.710	5.716	-81.910	-129.559	16.919		
400	57.948	314.780	295.681	8.594	-84.092	-135.385	15.715		
500	58.591	320.920	291.903	11.508	-126.417	-131.167	14.330		
600	59.544	331.692	302.662	17.418	-126.529	-139.307	12.128		
700	60.192	330.692	307.484	23.407	-126.669	-141.425	10.553		
800	60.648	348.997	312.179	30.621	-126.931	-143.513	9.370		
900	60.977	356.155	316.675	35.532	-127.222	-145.569	8.449		
1000	61.222	362.593	320.950	41.643	-127.606	-147.587	7.709		
1100	61.408	368.437	325.005	47.775	-128.061	-149.563	7.102		
1200	61.552	373.787	328.851	53.923	-128.504	-151.495	6.594		
1300	61.657	378.718	332.499	60.084	-129.243	-153.377	6.163		
1400	61.739	383.292	335.966	66.256	-129.991	-155.206	5.791		
1500	61.834	387.553	339.265	72.432	-130.859	-156.978	5.466		
1600	61.895	391.548	342.409	78.622	-146.395	-158.162	5.163		
1700	61.947	395.302	345.411	84.814	-147.137	-158.875	4.882		
1800	61.990	398.844	348.282	91.010	-147.961	-159.542	4.630		
1900	62.027	402.197	351.032	97.212	-148.871	-160.161	4.403		
2000	62.059	403.379	353.671	103.417	-149.870	-160.730	4.198		
2100	62.086	408.408	356.206	109.624	-150.955	-161.246	4.011		
2200	62.110	412.026	360.645	115.834	-152.121	-161.710	3.839		
2300	62.131	414.058	360.994	120.046	153.361	-162.118	3.682		
2400	62.149	416.702	363.261	128.250	154.666	-162.471	3.536		
2500	62.165	419.240	365.450	134.476	156.025	-162.768	3.401		
2600	62.180	421.678	367.566	140.693	157.425	-163.010	3.275		
2700	62.193	424.025	369.614	146.911	158.836	-163.198	3.157		
2800	62.204	426.287	371.598	153.131	151.264	-167.110	2.931		
2900	62.214	428.470	373.521	159.352	152.521	-165.597	2.841		
3000	62.224	430.580	373.388	165.574	152.039	-136.071	2.369		
3100	62.232	432.620	377.202	171.797	-152.594	-125.533	2.115		
3200	62.240	434.596	378.965	178.024	-152.718	-114.984	1.877		
3300	62.247	436.511	380.860	184.245	-153.008	-104.425	1.653		
3400	62.253	438.370	382.349	190.470	-153.259	-93.838	1.442		
3500	62.259	440.174	383.976	196.696	-153.471	-83.284	1.243		
3600	62.265	441.928	385.561	202.922	-153.641	-72.705	1.055		
3700	62.274	443.634	387.108	209.149	-153.769	-62.122	0.877		
3800	62.278	445.295	388.617	215.376	-153.858	-51.535	0.708		
3900	62.282	446.913	390.091	221.603	-153.907	-40.947	0.548		
4000	62.286	448.489	391.532	227.831	-153.920	-30.358	0.396		
4100	62.286	450.027	392.940	234.060	-153.898	-19.770	0.252		
4200	62.289	451.528	394.317	240.289	-153.844	-9.187	0.114		
4300	62.292	452.994	395.664	246.521	-153.763	-1.404			
4400	62.295	454.426	396.984	252.747	-153.656	11.939	-0.142		
4500	62.298	455.826	398.276	258.977	-153.528	22.570	-0.262		
5100	62.311	461.625	405.515	296.360	-152.406	-107.097	-0.970		
5200	62.313	464.835	406.644	302.591	-152.311	-96.544	-0.970		
5300	62.315	466.022	407.753	308.822	-152.129	-84.934	-0.591		
5400	62.316	467.186	408.843	315.034	-151.934	-128.193	-1.217		
5500	62.318	468.330	409.914	321.286	-151.788	-64.863	-0.691		
5600	62.319	469.453	410.967	327.518	-151.533	138.737	-1.294		
5700	62.321	470.556	412.003	333.750	-151.490	149.278	-1.368		
5800	62.322	471.640	413.022	341.982	-151.362	159.817	-1.439		
5900	62.323	472.705	414.025	346.214	-151.250	170.353	-1.508		
6000	62.324	473.752	415.011	352.446	-151.154	180.888	-1.575		

Beryllium Iodide (BeI<sub>2</sub>)

PREVIOUS December 1975 (1 atm)

Be<sub>1</sub>N<sub>1</sub>(C)

$M_r = 23.01888$  Beryllium Nitride (BeN)

$$S^\circ(298.15\text{ K}) = [208.77] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(0\text{ K}) = [424] \text{ kJ}\cdot\text{mol}^{-1}$$

Electronic Levels and Multiplicities	$\epsilon$ , cm <sup>-1</sup>	$g$ ,	[4]
state [1]	0		

$$\begin{aligned}\omega_c &= [1194] \text{ cm}^{-1} & \omega_c x_t &= [12.4] \text{ cm}^{-1} & \sigma &= 1 \\ B_c &= [1.555] \text{ cm}^{-1} & \alpha_c &= [0.019] & r_c &= [1.406] \text{ \AA}\end{aligned}$$

## Enthalpy of Formation

**Want Conviction? Add Satisfaction!**

**Heat Capacity and Entropy** The molecular constants were taken from Gordon.<sup>1</sup>

#### Reference

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IDEAL-GAS

$M = 23$  01888 Beyllium Nitride (BeN)

$$\Delta H^\circ(0\text{ K}) = [424] \text{ kJ}\cdot\text{mol}^{-1}$$

Enthalpy Reference Temperature =  $T_r = 298.15\text{ K}$  Standard State Pressure =  $p^{\circ}$   
 $= [424]\text{ kJ}\cdot\text{mol}^{-1}$        $\text{K}^{-1}\cdot\text{mol}^{-1}$        $\text{kJ}\cdot\text{mol}^{-1}$

PREVIOUS TIME		CURRENT TIME	
TIME	STATE	TIME	STATE
-6...	INFINITE	424.231	424.231
0...	0...	428.231	428.231
0...	0...	476.725	476.645
100...	29.111	23.965	-5.821
200...	29.254	16.758	211.487
250...	29.583	16.957	209.260
298.15	30.089	208.768	208.768
300	30.111	208.954	208.768
350	30.757	213.643	209.137
400	31.439	217.794	209.964
450	32.102	221.536	211.046
500	32.716	224.951	212.064
600	33.761	231.012	214.900
700	34.574	237.280	217.586
800	35.203	240.939	220.219
900	35.693	245.115	227.758
1000	36.081	248.897	225.185
1100	36.395	252.351	227.500
1200	36.633	258.529	229.705
1300	36.869	258.471	231.806
1400	37.052	261.211	233.810
1500	37.211	263.772	235.723
1600	37.351	266.179	237.552
1700	37.475	268.447	239.303
1800	37.587	270.592	240.982
1900	37.689	272.627	242.595
2000	37.783	274.553	244.145
2100	37.870	276.408	245.638
2200	37.951	278.172	247.077
2300	38.027	280.860	248.466
2400	38.100	281.480	249.808
2500	38.169	283.037	251.106
2600	38.226	284.515	252.363
2700	38.300	285.980	253.582
2800	38.361	287.374	254.764
2900	38.421	288.721	255.912
3000	38.479	290.024	257.027
3100	38.516	291.287	258.113
3200	38.552	292.511	259.168
3300	38.646	293.700	260.197
3400	38.700	294.834	261.199
3500	38.752	295.977	262.177
3600	38.804	297.099	263.131
3700	38.855	298.133	264.063
3800	38.906	299.170	264.973
3900	38.956	300.181	265.863
4000	39.005	301.168	266.733
4100	39.054	302.120	267.585
4200	39.102	303.074	268.419
4300	39.151	303.994	269.225
4400	39.198	304.895	270.035
4500	39.246	305.776	270.820
5000	39.525	310.706	275.228
5200	39.571	311.474	275.918
4600	39.293	306.639	271.589
4700	39.340	307.485	272.344
4800	39.387	308.314	273.085
4900	39.433	309.216	273.812
5000	39.479	309.923	274.526
5100	39.525	310.706	275.304
5200	39.571	311.474	275.980
5300	39.617	312.228	276.596
5400	39.662	312.969	277.262
5500	39.708	313.697	277.918
5600	39.753	314.413	278.564
57000	39.798	315.111	279.209
58000	39.843	315.809	279.824
59000	39.888	316.491	280.446
60000	39.933	317.162	281.046

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Beryllium Oxide, Alpha ( $\alpha$ -BeO)CRYSTAL( $\alpha$ )CRYSTAL( $\alpha$ ) $\text{Be}_1\text{O}_1(\text{cr})$ 

$$\Delta H^\circ(0 \text{ K}) = 13.770 \pm 0.21 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_d H^\circ(298.15 \text{ K}) = -608.4 \pm 3.3 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_{\text{irr}} H^\circ = [6.694 \pm 1.7] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_{\text{lo}} H^\circ = [79.057 \pm 6.3] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_{\text{lo},\text{f}} H^\circ = 84.9 \pm 6.3 \text{ kJ}\cdot\text{mol}^{-1}$$

## Enthalpy of Formation

Parker thoroughly reviewed the data as of 1969 and selected  $-145.4 \pm 0.8 \text{ kcal}\cdot\text{mol}^{-1}$ . She later revised<sup>1</sup> this value to  $-145.7 \pm 0.6 \text{ kcal}\cdot\text{mol}^{-1}$  due to new HF-solution calorimetry on  $\text{BeF}_3$ (amorphous) performed by Kilday *et al.*<sup>2</sup> Values of  $\Delta H^\circ$  from Parker's revised analysis<sup>3</sup> are summarized below. We adopt  $-145.4 \pm 0.8$ , rather than the revised selection, as a compromise between the indirect results based on  $\text{Be}(\text{cr})$  and those based on  $\text{BeF}_3(\text{am})$ . The latter depend on  $\Delta H^\circ$  for  $\text{HF}(\text{n H}_2\text{O})$ . Use of the JANAF  $\Delta H^\circ$ <sup>4</sup> in place of the NBS value<sup>5</sup> causes a change of  $\pm 0.9 \text{ kcal}\cdot\text{mol}^{-1}$  in the results based on  $\text{BeF}_3(\text{am})$ . Recent data for HF suggest that the change could be even larger.

Direct Determination of  $\Delta H^\circ$ Indirect Determinations of  $\Delta H^\circ$ 

## Source

keal·mol<sup>-1</sup>keal·mol<sup>-1</sup>

## Source

keal·mol<sup>-1</sup>

## Beryllium Oxide, Beta ( $\beta$ -BeO)

### CRYSTAL( $\beta$ )

### $M_r = 25.01158$ Beryllium Oxide, Beta (BeO)

$$\begin{aligned} S^o(298.15\text{ K}) &= [16.5911\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}] \\ T_{\text{in}} &= 2373 \pm 15\text{ K } (\alpha \rightarrow \beta) \\ T_{\text{fin}} &= [2821.2 \pm 100]\text{ K } (\beta \rightarrow \beta) \end{aligned}$$

#### Enthalpy of Formation

$\Delta_f H^\circ$  is calculated from that of BeO( $\alpha$ , cr) by addition of  $\Delta_{\text{cr}}H^\circ$ , since the difference in enthalpy,  $H^\circ(298.15\text{ K}) - H^\circ(298.15\text{ K})$ , between the  $\alpha$ - and  $\beta$ -phases is zero according to the adopted functions.

#### Heat Capacity and Entropy

$C_p^o$  is taken to be the same as that of BeO( $\alpha$ , cr). Enthalpy data for  $\beta$ -BeO<sup>1</sup> extend from 2377 to 2501 K, a range too short for obtaining an accurate  $C_p^o$  curve. The enthalpy data deviate from the adopted functions by  $-0.2$  to  $\pm 1.4\%$ . Other enthalpy data<sup>2-4</sup> show no obvious transition to  $\beta$ -BeO; this suggests that experimental uncertainties masked the transition or that these samples failed to transform.  $S^o$  is calculated in a manner analogous to that used for  $\Delta_f H^\circ$ .

#### Transition Data

Studies of x-ray diffraction,<sup>5-7</sup> optical properties,<sup>6,8</sup> thermal expansion,<sup>1,9</sup> thermal analysis,<sup>10-14</sup> enthalpy,<sup>1</sup> and decrepitation of single crystals<sup>6,9,15</sup> indicate the existence of a reversible transition near 2100°C.  $\beta$ -BeO is tetragonal with a structure related to rutile,<sup>5</sup> while  $\alpha$ -BeO is hexagonal close-packed with a wurtzite-type structure.<sup>16,17</sup>

$T_{\text{in}}$  is lower than cooling than on heating. Earlier studies gave temperature differences of about 40°, 11, 12, 50°<sup>7</sup> and 80°<sup>14</sup>, but a recent DTA study<sup>10</sup> gave  $T_{\text{in}}$  values on cooling which were only  $\sim 15^\circ$  below those on heating.  $T_{\text{in}} = 2107 \pm 7^\circ\text{C}$  (IPTS-68) was proposed as a DTA standard temperature because it is reproducible and relatively unchanged by oxide impurities.<sup>10</sup> Reported values of  $T_{\text{in}}$  on heating include 2100  $\pm$  10°C,<sup>1</sup> 2107  $\pm$  7°C,<sup>10</sup> 2095°C,<sup>11</sup> 2075  $\pm$  15°C,<sup>12</sup> 2050–2250°C,<sup>7</sup> 2144  $\pm$  40°C,<sup>14</sup> and 2050  $\pm$  25°C.<sup>6</sup> We adopt 2100  $\pm$  15°C.

Reported values of  $\Delta_{\text{cr}}H^\circ$  include  $1.35 \pm 0.1$ ,<sup>1</sup>  $1.40 \pm 0.25$ ,<sup>10</sup>  $1.25 \pm 0.25$ ,<sup>14</sup> and  $0.95 \pm 0.3$  kcal·mol<sup>-1</sup>.<sup>13</sup> The first value is from enthalpy data and the others are from thermal analysis. It is not clear why the transition fails to appear in two other enthalpy studies.<sup>12</sup> We adopt  $\Delta_{\text{cr}}H^\circ = 1.60 \pm 0.4$  kcal·mol<sup>-1</sup> derived from the difference between the enthalpy data for  $\beta$ -BeO<sup>1</sup> and the JANAF enthalpy for  $\alpha$ -BeO.

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### CRYSTAL( $\beta$ )

### $M_r = 25.01158$ Beryllium Oxide, Beta (BeO)

$$\begin{aligned} \Delta_f H^\circ(298.15\text{ K}) &= [-601.659] \text{ kJ}\cdot\text{mol}^{-1} \\ \Delta_{\text{cr}}H^\circ &= 6.694 \pm 1.7 \text{ kJ}\cdot\text{mol}^{-1} \\ \Delta_{\text{cr}}H^\circ &= [79.057 \pm 6.3] \text{ kJ}\cdot\text{mol}^{-1} \end{aligned}$$

#### Enthalpy of Formation

$\Delta_f H^\circ$  is calculated from that of BeO( $\alpha$ , cr) by addition of  $\Delta_{\text{cr}}H^\circ$ , since the difference in enthalpy,  $H^\circ(298.15\text{ K}) - H^\circ(298.15\text{ K})$ , between the  $\alpha$ - and  $\beta$ -phases is zero according to the adopted functions.

#### Heat Capacity and Entropy

$C_p^o$  is taken to be the same as that of BeO( $\alpha$ , cr). Enthalpy data for  $\beta$ -BeO<sup>1</sup> extend from 2377 to 2501 K, a range too short for obtaining an accurate  $C_p^o$  curve. The enthalpy data deviate from the adopted functions by  $-0.2$  to  $\pm 1.4\%$ . Other enthalpy data<sup>2-4</sup> show no obvious transition to  $\beta$ -BeO; this suggests that experimental uncertainties masked the transition or that these samples failed to transform.  $S^o$  is calculated in a manner analogous to that used for  $\Delta_f H^\circ$ .

#### Transition Data

Studies of x-ray diffraction,<sup>5-7</sup> optical properties,<sup>6,8</sup> thermal expansion,<sup>1,9</sup> thermal analysis,<sup>10-14</sup> enthalpy,<sup>1</sup> and decrepitation of single crystals<sup>6,9,15</sup> indicate the existence of a reversible transition near 2100°C.  $\beta$ -BeO is tetragonal with a structure related to rutile,<sup>16,17</sup> is hexagonal close-packed with a wurtzite-type structure.<sup>16,17</sup>

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#### Transition Data

## LIQUID

 $M_r = 25.01158$  Beryllium Oxide (BeO)

## Beryllium Oxide (BeO)

$$\begin{aligned}S^{\circ}(298.15 \text{ K}) &= [35.931] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1} \\T_{\text{fus}} &= [2821.2 \pm 100] \text{ K } (\beta - 1) \\T_{\text{fus}} &= 2780 \pm 100 \text{ K } (\alpha \rightarrow 1)\end{aligned}$$

## Enthalpy of Formation

$\Delta_f H^\circ$  is calculated from that of  $\alpha$ -BeO by adding  $\Delta_{\text{fus}}H^\circ$  and the difference in enthalpy,  $H^\circ(2780 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the  $\alpha$  and liquid phases.

## Heat Capacity and Entropy

$C_p^\circ$  is taken to be  $19 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , based on the lower two of three enthalpy points ( $2867$ – $3159 \text{ K}$ ) measured by Shpil'rain *et al.*<sup>1</sup>. The upper two points yield  $24.9 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , which is too large in our opinion. Earlier enthalpy data<sup>2</sup>, are inadequate for deriving  $C_p^\circ$ . Below the assumed glass transition at  $1900 \text{ K}$ ,  $C_p^\circ$  is taken to be the same as that of the crystal.  $S^\circ$  is calculated in a manner analogous to that used for  $\Delta_f H^\circ$ .

## Fusion Data

Conflicting evidence suggests that the melting points of  $\alpha$ - and  $\beta$ -BeO are quite uncertain. Schneider's review<sup>4</sup> listed C six values ( $T_{\text{fus}}$ )<sup>°C</sup>, IPTS-48, with dates in parentheses)  $24.0(1916)$ ,  $2452(1956)$ ,  $2508(1937)$ ,  $2557(1930)$ ,  $2570(1948)$  and  $2573^{\circ}$ – $1913$ ). Subsequent  $T_{\text{fus}}$  values include  $2430 \pm 10^{\circ}$ ,  $2560 \pm 10^{\circ}$ ,  $2544 \pm 30^{\circ}$ ,  $2547 \pm 9^{\circ}$ ,  $2450 \pm 30$  and  $2470 \pm 30^{\circ}\text{C}$ . The reported values fall roughly into two groups near  $2450^{\circ}\text{C}$  and  $2560^{\circ}\text{C}$ . Three enthalpy studies<sup>1–3</sup> avoided the region from  $2435^{\circ}\text{C}$  to  $2547^{\circ}\text{C}$ . Part of the conflict arises because, in most cases, the measurement of  $T_{\text{fus}}$  of BeO was only an incidental part of the study. Such values are more likely to be in error due to temperature measurement, detection of melting, impurities, volatilization and reaction with the surroundings. The actual discrepancies may be even larger than they appear, since one of the higher  $T_{\text{fus}}$  values seems to refer to  $\alpha$ -BeO which should melt  $\sim 40$  below  $\beta$ -BeO. Enthalpy data of Kandyba *et al.*<sup>2</sup> suggest that their sample may have remained as  $\alpha$ -BeO, yet they reported  $T_{\text{fus}} = 2547 \pm 9^{\circ}\text{C}$ . In contrast  $T_{\text{fus}} = 2430 \pm 10^{\circ}\text{C}$  was found for  $\beta$ -BeO by Latta *et al.*<sup>3</sup>; their thermal analysis showed both  $T_{\text{m}}$  and  $T_{\text{fus}}$ .

The conflict is epitomized by the two most recent values of  $T_{\text{fus}}$ :  $2430 \pm 10^{\circ}\text{C}$ <sup>4</sup> and  $2560 \pm 10^{\circ}\text{C}$ <sup>5</sup>. These studies<sup>5,6</sup> seem to be more satisfactory than their predecessors yet at least one of them has a large bias. They agree<sup>5,6</sup> on  $T_{\text{fus}}$  for  $\text{Al}_2\text{O}_3$ ,  $\text{Mn}$  and  $\text{Ta}$  but differ in opposite directions for  $\text{BeO}$  and  $\text{UO}_2$ . Non-stoichiometry could explain the lower  $T_{\text{fus}}(\text{UO}_2)$  reported by Riley<sup>6</sup>, but analogous evidence for BeO is lacking. As a compromise, we adopt  $T_{\text{fus}}(\text{BeO}) = 2507^{\circ}\text{C} = 2780 \text{ K}$  and calculate  $T_{\text{fus}}(\text{BeO}) = 2821.2 \text{ K}$  from  $\Delta_f G^\circ = 0$  for  $\text{BeO}(\beta) \rightarrow \text{BeO}(\text{l})$ .

$\Delta_f H^\circ(\text{c}) = 20.3 \text{ kcal}\cdot\text{mol}^{-1}$  is calculated by difference from enthalpies ( $2867$ – $3159 \text{ K}$ ) of Shpil'rain *et al.*<sup>1</sup>, and the JANAF enthalpy for  $\alpha$ -BeO. We assume that BeO(I) reverts to  $\alpha$ -BeO and that  $\beta$ -BeO did not form during the drop calorimetry.<sup>1</sup>  $\Delta_{\text{fus}}H^\circ(\beta) = 13.895 \text{ kcal}\cdot\text{mol}^{-1}$  is calculated from  $\text{BeO}(\text{B}) \rightarrow \text{BeO}$  at the corresponding  $T_{\text{fus}}$  using the adopted tables. Enthalpy data of Greenbaum *et al.*<sup>3</sup> gave  $\Delta_{\text{fus}}H^\circ = 19.3 \text{ kcal}\cdot\text{mol}^{-1}$  (phase uncertain) even though both the crystal and liquid data have large negative bias. Ohta and Sato<sup>7</sup> derived  $\Delta_{\text{fus}}H^\circ = 7.6 \pm 2.1 \text{ kcal}\cdot\text{mol}^{-1}$  from liquidus data in the binary system  $\text{BeO}-\text{ThO}_2$ . This can be discounted along with other binary data<sup>8,9,10</sup>, due to the uncertainty in  $T_{\text{fus}}$ .

## Vaporization Data

The vapor over BeO is composed mainly of trimer, tetramer and individual atoms, along with minor amounts of several other molecules.

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$M_r = 25.01158$ Beryllium Oxide (BeO)		$M_r = 25.01158$ Beryllium Oxide (BeO)	
		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$	
		$T/K$	$C_p^\circ$
0			
298.15	25.560	35.931	35.931
200	25.744	36.089	35.931
300	33.757	44.675	37.047
400	38.200	52.002	39.596
500	42.376	60.222	42.259
600	44.823	64.948	51.313
800	46.656	70.058	48.405
900	48.091	78.539	51.459
1000	49.262	83.768	54.437
1100	50.254	88.511	57.322
1200	51.116	92.921	60.107
1300	51.882	97.093	62.791
1400	52.580	101.914	63.577
1500	53.225	104.564	67.869
1600	53.827	108.018	70.272
1700	54.396	111.399	72.389
1800	54.944	114.423	74.527
1900	55.467	117.408	76.794
1900.001	55.467	117.408	76.794
1900.001	59.496	117.408	76.794
2000	79.496	121.486	79.114
2100	79.496	125.364	81.225
2200	79.496	129.063	83.316
2300	79.496	132.596	85.382
2400	79.496	135.980	87.421
2500	79.496	139.225	89.428
2600	79.496	142.343	91.404
2700	79.496	145.343	93.346
2800	79.496	148.234	95.255
2821.20	79.496	148.334	95.656
2900	79.496	151.024	97.131
3000	79.496	153.719	98.972
3100	79.496	156.525	100.780
3200	79.496	158.349	102.556
3300	79.496	161.295	104.299
3400	79.496	163.669	106.077
3500	79.496	165.973	107.691
3600	79.496	168.213	109.341
3700	79.496	170.391	110.962
3800	79.496	172.511	112.554
3900	79.496	174.576	114.118
4000	79.496	176.588	115.654
4100	79.496	178.551	117.165
4200	79.496	180.467	118.649
4300	79.496	182.337	120.109
4400	79.496	184.165	121.544
4500	79.496	185.952	122.955
4600	79.496	187.699	124.344
4700	79.496	189.408	125.710
4800	79.496	191.082	127.055
4900	79.496	192.721	128.378
5000	79.496	194.327	129.681

$M_r = 25.01158$ Beryllium Oxide (BeO)		Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$	
		$T/K$	$C_p^\circ$
0			
100	0.4	0.047	-542.705
200	0.47	0.047	-542.715
300	0.51	0.051	-543.039
400	0.55	0.055	-544.397
500	0.59	0.059	-545.761
600	0.63	0.063	-547.129
700	0.67	0.067	-548.481
800	0.71	0.071	-549.444
900	0.75	0.075	-549.931
1000	0.79	0.079	-551.021
1100	0.83	0.083	-551.626
1200	0.87	0.087	-552.704
1300	0.91	0.091	-553.387
1400	0.95	0.095	-553.637
1500	0.99	0.099	-553.934
1600	1.03	0.103	-554.113
1700	1.07	0.107	-554.291
1800	1.11	0.111	-554.469
1900	1.15	0.115	-554.647
2000	1.19	0.119	-554.825
2100	1.23	0.123	-555.003
2200	1.27	0.127	-555.181
2300	1.31	0.131	-555.359
2400	1.35	0.135	-555.537
2500	1.39	0.139	-555.715
2600	1.43	0.143	-555.893
2700	1.47	0.147	-556.071
2800	1.51	0.151	-556.249
2821.2	1.55	0.155	-556.427
2900	1.59	0.159	-556.605
3000	1.63	0.163	-556.783
3100	1.67	0.167	-556.961
3200	1.71	0.171	-557.139
3300	1.75	0.175	-557.317
3400	1.79	0.179	-557.495
3500	1.83	0.183	-557.673
3600	1.87	0.187	-557.851
3700	1.91	0.191	-558.029
3800	1.95	0.195	-558.207
3900	1.99	0.199	-558.385
4000	2.03	0.203	-558.563
4100	2.07	0.207	-558.741
4200	2.11	0.211	-558.919
4300	2.15	0.215	-559.097
4400	2.19	0.219	-559.275
4500	2.23	0.223	-559.453
4600	2.27	0.227	-559.631
4700	2.31	0.231	-559.809
4800	2.35	0.235	-559.987
4900	2.39	0.239	-560.165
5000	2.43	0.243	-560.343

$M_r = 25.01158$ Beryllium Oxide (BeO)		Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$	
		$T/K$	$C_p^\circ$
0			
100	0.4	0.047	-542.705
200	0.47	0.047	-542.715
300	0.51	0.051	-543.039
400	0.55	0.055	-544.397
500	0.59	0.059	-545.761
600	0.63	0.063	-547.129
700	0.67	0.067	-548.481
800	0.71	0.071	-549.444
900	0.75	0.075	-550.521
1000	0.79	0.079	-551.599
1100	0.83	0.083	-552.677
1200	0.87	0.087	-553.755
1300	0.91	0.091	-554.833
1400	0.95	0.095	-555.911
1500	0.99	0.099	-556.989
1600	1.03	0.103	-558.067
1700	1.07	0.107	-559.145
1800	1.11	0.111	-559.223
1900	1.15	0.115	-559.301
2000	1.19	0.119	-559.379
2100	1.23	0.123	-559.457
2200	1.27	0.127	-559.535
2300	1.31	0.131	-559.613
2400	1.35	0.135	-559.691
2500	1.39	0.139	-559.769
2600	1.43	0.143	-559.847
2700	1.47	0.147	-559.925
2800	1.51	0.151	-560.003
2821.2	1.55	0.155	-560.081
2900	1.59	0.159	-560.159
3000	1.63	0.163	-560.237
3100	1.67	0.167	-560.315
3200	1.71	0.171	-560.393
3300	1.75	0.175	-560.471
3400	1.79	0.179	-560.549
3500	1.83	0.183	-560.627
3600	1.87	0.187	-560.705
3700	1.91	0.191	-560.783
3800	1.95	0.195	-560.861
3900	1.99	0.199	-560.939
4000	2.03	0.203	-561.017
4100	2.07	0.207	-561.095
4200	2.11	0.211	-561.173
4300	2.15	0.215	-561.251
4400	2.19	0.219	-561.329
4500	2.23	0.223	-561.407
4600	2.27	0.227	-561.485

## Beryllium Oxide (BeO)

### M<sub>r</sub> = 25.01158 Beryllium Oxide (BeO)

#### CRYSTAL( $\alpha$ - $\beta$ )-LIQUID

0 to 2373 K crystal, alpha  
2373 to 2821.2 K crystal, beta  
above 2821.2 K liquid

Refer to the individual tables for details.

#### Be<sub>1</sub>O<sub>1</sub>(cr, l)

T/K	C <sub>p</sub> J·K <sup>-1</sup> ·mol <sup>-1</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa	
		S <sup>o</sup> J·K <sup>-1</sup>	-[G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ) kJ·mol <sup>-1</sup>	Δ <sub>i</sub> H <sup>o</sup> kJ·mol <sup>-1</sup>
0	0	0	0	-2335	-604.914
100	2.636	0.824	28.539	-605.343	-604.914
200	14.159	5.887	15.759	-1.974	-597.709
298.15	25.560	13.770	13.770	0	-598.573
300	25.744	13.928	13.770	0.047	-598.354
400	33.757	23.513	14.886	3.051	-598.880
500	36.920	30.641	17.235	6.703	-598.922
600	42.376	38.061	20.098	10.778	-598.668
700	44.823	44.286	21.152	15.144	-598.440
800	46.656	50.897	26.244	19.722	-598.310
900	48.091	56.478	29.298	24.462	-597.666
1000	49.262	61.607	32.276	29.331	-597.073
1100	50.254	66.350	35.161	34.308	-596.329
1200	51.116	70.760	37.946	39.377	-595.592
1300	51.882	74.882	40.630	44.327	-595.815
1400	52.580	78.753	43.216	49.751	-595.994
1500	53.225	82.403	45.708	55.042	-594.744
1600	53.827	85.857	48.111	60.394	-594.971
1700	54.396	89.138	50.428	65.806	-595.303
1800	54.944	92.262	52.666	71.273	-595.761
1900	55.467	95.247	54.829	76.794	-596.904
2000	55.974	98.105	56.922	82.366	-597.176
2100	56.467	100.848	58.949	87.988	-595.330
2200	56.948	103.486	60.914	93.659	-594.669
2300	57.421	106.028	62.820	99.378	-594.893
2373.001	57.756	107.827	64.177	103.582	ALPHA <-> BETA
2373.001	57.758	110.649	64.177	110.276	TRANSITION
2400	57.881	111.303	64.704	111.837	-605.409
2500	58.338	113.675	66.616	117.648	-603.605
2600	58.789	115.972	68.470	123.504	-602.605
2700	59.233	118.199	70.278	129.406	-603.959
2800	59.676	120.361	72.021	135.351	-604.074
2821.220	59.770	120.812	72.386	136.618	BETA <-> LIQUID
2821.220	59.496	148.834	72.386	215.676	TRANSITION
2900	79.496	151.024	74.493	221.939	-606.409
3000	79.496	151.719	77.089	229.888	-607.695
3100	79.496	156.325	79.603	237.838	-603.847
3200	79.496	158.849	82.041	253.787	-600.016
3300	79.496	161.295	84.405	253.737	-796.202
3400	79.496	163.669	86.702	792.408	-238.007
3500	79.496	165.973	88.934	269.636	-122.149
3600	79.496	168.213	91.105	277.586	-221.149
3700	79.496	170.391	93.219	285.535	-224.402
3800	79.496	172.511	95.278	293.485	-227.073
3900	79.496	174.576	97.285	301.435	-230.007
4000	79.496	176.588	99.242	309.384	-233.767
4100	79.496	178.551	101.153	317.334	-237.334
4200	79.496	180.467	103.018	325.283	-241.402
4300	79.496	182.337	104.841	333.233	-245.403
4400	79.496	184.165	106.624	341.183	-249.497
4500	79.496	185.952	108.567	349.132	-252.431
4600	79.496	187.699	110.072	357.082	-258.007
4700	79.496	189.408	111.742	365.031	-265.550
4800	79.496	191.082	113.378	372.981	-272.909
4900	79.496	192.721	114.980	380.931	-280.246
5000	79.496	194.327	116.551	388.380	-285.761

CURRENT December 1974

PREVIOUS

#### Be<sub>1</sub>O<sub>1</sub>(cr, l)

IDEAL GAS

## Beryllium Oxide (BeO)

$M_r = 25.01158$  Beryllium Oxide (BeO)

Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$												Standard State Pressure = $p^* = 0.1 \text{ MPa}$						
						$\frac{C_p}{\text{J K}^{-1} \cdot \text{mol}^{-1}}$						$\frac{H^* - H^*(T_r)}{\text{J K}^{-1} \cdot \text{mol}^{-1}}$						
						$\frac{S^* - [G^* - H^*(T_r)]/T}{\text{J K}^{-1}}$						$\Delta H^*$						
Source	State	$\epsilon, \text{cm}^{-1}$	$g,$	Electronic and Molecular Constants ( $\sigma = 1$ )		$B, \text{cm}^{-1}$	$\alpha, \text{cm}^{-1}$	$\omega_{\text{ce}}, \text{cm}^{-1}$	$\omega_{\text{e}}, \text{cm}^{-1}$	$\omega_{\text{ce}}, \text{cm}^{-1}$		$T/K$	$C_p^*$	$S^*$	$H^* - H^*(T_r)/T$	$\Delta G^*$	$\log K_r$	
1	X <sup>+</sup>	0.0	1	1.3310	1.6510	0.0190	1487.3	11.83			0	100	29.108	165.763	223.160	-8.988	133.984	INFINITE
1-7	X <sup>+</sup>	[8000]	6	[1.463]	[1.366]	[0.0163]	[130.8]	8.2			200	29.139	185.943	200.307	-2.873	127.536	-66.118	
1	A <sup>1\Pi</sup>	9234.8	2	1.4632	1.3661	0.0163	1144.2	8.42			298.15	29.481	197.625	0.	136.398	31.150	-31.150	
4	A <sup>1\Sigma</sup>	[16000]	3	[1.362]	[1.576]	[0.015]	[7.8]				300	29.493	197.807	197.626	0.055	110.873	-19.425	
1	A <sup>1\Pi</sup>	21197.	1	1.3623	1.5758	0.0154	1370.8	7.75			400	30.493	206.400	198.791	3.043	136.395	10.715	-10.715
4	A <sup>1\Sigma</sup>	[37000]	3	[1.49]	[1.31]	[0.01]	[1082]	[9.]			500	31.421	213.286	201.023	6.131	135.513	102.198	-13.346
4	A <sup>1\Pi</sup>	[38000]	6	[1.49]	[1.31]	[0.01]	[1082]	[9.]			1000	35.252	236.418	213.490	53.465	131.569	93.793	-9.793
1	D <sup>1\Delta</sup>	38918.	2	1.49	1.31	0.01	1081.5	9.1			1100	35.784	239.803	215.750	26.480	130.595	93.793	-9.793
1-4	S <sup>1\Sigma</sup>	[40000]	3	[1.49]	[1.31]	[0.01]	[1012.2]	8.4			1200	36.357	242.941	217.869	30.086	129.569	38.079	-1.655
1-4	S <sup>1\Sigma</sup>	38956.	1	[1.49]	[1.31]	[0.01]	[1082]	[9.]			1400	37.023	248.876	219.911	33.755	127.403	-1.223	-5.771
4	S <sup>1\Sigma</sup>	[47000]	1	[1.49]	[1.31]	[0.01]	[1082]	[9.]			1500	38.788	251.290	223.740	41.325	126.291	-0.856	-0.540

Enthalpy of Formation

We adopt  $D_B^0 = 104.2 \pm 3$  and  $\Delta H^\circ(298.15\text{ K}) = -37.6 \pm 3$  kcal mol<sup>-1</sup> based on two mass-spectrometric studies,<sup>10</sup> analyzed below. The adopted values correspond to the average of the two results for reaction A and also to the average for reaction B. Improved agreement between reactions A and B is due to recalculation of  $K_p$  of reaction B using the current table<sup>11</sup> for BeO(*o*). Our analysis should be compared to the analysis of Brewer and Rosenblatt,<sup>10</sup> using "functions based upon calculated levels."

Heat Capacity and Entropy

Electronic levels ( $T_0$ ) and vibrational-rotational constants of the observed states are from Rosen. Field<sup>1</sup> concluded that calculations<sup>2,3</sup> of the isoconfigurational A'II - II separation should be adequate for estimating the low-lying  $\Pi$  state. The adopted separation of  $1200 \text{ cm}^{-1}$  is consistent with analysis<sup>4</sup> of perturbations. We estimate  $\zeta_{\Sigma}$  at  $16000 \text{ cm}^{-1}$  by assuming that it lies  $5200 \pm 4000 \text{ cm}^{-1}$  below the isoconfigurational B state. Other predicted states and their vibrational-rotational constants are facilitated by listing the states in the isoconfigurational order of MgO. Our thermodynamic functions correspond to an "effective" ground state with  $g = 2$  instead of  $g = 3$  or 4 in Eq. (1). This comparison is only approximate since our functions are calculated using first-order anharmonic corrections to Q<sub>i</sub> and Q'<sub>i</sub> in the partition function  $Q = Q_{\Sigma} / [Q_{\Sigma} + Q_i e^{\beta E_i}]$ .

Sublimation and Vaporization Data

Mass spectra<sup>8,9</sup> at 1900–2400 K showed the vapor to consist mainly of Be, O, (BeO)<sub>3</sub>, and (BeO), and other polymer of BeO. Tetramer, trimer and pentamer become dominant at higher temperatures.

with small amounts of O<sub>2</sub>, Be<sub>2</sub>O, BeO

and other polymer of BeO. Tetramer, trimer and pentamer become dominant at higher temperatures.

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## Beryllium Oxide (BeO)

Continued on page 428

**B<sub>2</sub>O<sub>3</sub>S<sub>1</sub>(cr)****M<sub>r</sub> = 105.06978 Beryllium Sulfate, Alpha (BeSO<sub>4</sub>)****CRYSTAL( $\alpha$ )**

		Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$				Standard State Pressure = $P^* = 0.1\text{ MPa}$			
		$\Delta H^\circ(0\text{ K}) = -1190.1 \pm 3.3\text{ kJ}\cdot\text{mol}^{-1}$				$\Delta H^\circ(298.15\text{ K}) = -1200.8 \pm 3.3\text{ kJ}\cdot\text{mol}^{-1}$			
		$\Delta_{m1}H^\circ = [1.1113]\text{ kJ}\cdot\text{mol}^{-1}$				$\Delta_{m2}H^\circ = [19.552]\text{ kJ}\cdot\text{mol}^{-1}$			
<b>Enthalpy of Formation</b>									
Bear <i>et al.</i> <sup>1</sup> measured the enthalpies of solution of Be(cr) and BeSO <sub>4</sub> (cr,a) in concentrated HF and the enthalpy of reaction of H <sub>2</sub> SO <sub>4</sub> (aq) with BeO <sub>2</sub> (aq) HF. Combination of these yields reaction (a) below. Taylor <i>et al.</i> <sup>2</sup> measured enthalpies of solution of Be(cr) and BeSO <sub>4</sub> (cr,a) in H <sub>2</sub> SO <sub>4</sub> (aq) which yields reaction (b). Marchal <sup>3</sup> measured the total vapor pressure of BeSO <sub>4</sub> (cr) in the temperature range 863–1103 K. Partial pressures of SO <sub>3</sub> (g) were calculated from Marchal's <sup>3</sup> data using $\Delta H^\circ$ values for the SO <sub>3</sub> –SO <sub>2</sub> equilibrium. 3rd law analysis of these data yields $\Delta H^\circ$ for reaction (c) as given below. This was converted to $\Delta H^\circ$ for $\alpha$ -BeSO <sub>4</sub> using JANAF enthalpies of transitions.		$\Delta H^\circ(298.15\text{ K})$	$\Delta H^\circ(298.15\text{ K})$	$\Delta H^\circ(298.15\text{ K})$	$\Delta H^\circ(298.15\text{ K})$	$\Delta H^\circ(298.15\text{ K})$	$\Delta H^\circ(298.15\text{ K})$	$\Delta H^\circ(298.15\text{ K})$	$\Delta H^\circ(298.15\text{ K})$
Source	Method	Reaction	T/K	$\Delta_{us}H_f$ kcal·mol <sup>-1</sup>	$\Delta_{us}H_f$ kJ·mol <sup>-1</sup>	$\Delta_{us}H_f$ kcal·mol <sup>-1</sup>	$\Delta_{us}H_f$ kJ·mol <sup>-1</sup>	$\Delta_{us}H_f$ kcal·mol <sup>-1</sup>	$\Delta_{us}H_f$ kJ·mol <sup>-1</sup>
1	Calorimetric	(a) Be(cr) + H <sub>2</sub> SO <sub>4</sub> (109 H <sub>2</sub> O) = H <sub>2</sub> (g) + $\alpha$ -BeSO <sub>4</sub>	294	-74.47	-286.65 ± 0.5	100	174.431	228.245	135.278
2	Calorimetric	(b) Be(cr) + H <sub>2</sub> SO <sub>4</sub> (47.849 H <sub>2</sub> O) = H <sub>2</sub> (g) + $\alpha$ -BeSO <sub>4</sub>	298	-76.38	-287.55 ± 0.13	100	183.088	245.296	144.510
3	$K_p$ (973–1083 K)	(c) BeSO <sub>4</sub> ( $\gamma$ ) → BeO(cr) + SO <sub>3</sub> (g)	298	43.92	-286.55 ± 0.5	1200	189.209	261.502	153.591
The adopted $\Delta H^\circ(298.15\text{ K}) = -287.0 \pm 0.8$ is an average value of reaction (a) and (b). This value is for relatively finely divided crystals of BeSO <sub>4</sub> as was indicated by Bear <i>et al.</i> <sup>1</sup>									
<b>Heat Capacity and Entropy</b>									
Low temperature heat capacities (12–301 K) and high temperature enthalpies (366–864 K) were measured by Taylor, Gardner and Smith. <sup>5</sup> These data were joined smoothly at 298.15 K and extrapolated graphically above 864 K. The entropy was obtained from the heat capacities using $S^\circ(12.56\text{ K}) = 0.034\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ .									

**Transition Data**

Bosik, Novoselova and Simanov<sup>6</sup> observed two endothermic effects at 863–883 K and 908–913 K on the heating and cooling curves of BeSO<sub>4</sub>(cr), thus we have adopted  $T_{m1}(\alpha \rightarrow \beta) = 863\text{ K}$  and  $T_{m2}(\beta \rightarrow \alpha) = 908\text{ K}$ .  $\Delta_{m1}H^\circ(\alpha \rightarrow \beta) = 0.266\text{ kcal}\cdot\text{mol}^{-1}$  was obtained from the single enthalpy point at 863.9 K observed by Taylor, Gardner and Smith,<sup>5</sup>  $\Delta_{m2}H^\circ(\beta \rightarrow \gamma) = 4.673\text{ kcal}\cdot\text{mol}^{-1}$  was chosen in order to give good agreement with the equilibrium data of Marchal.<sup>3</sup>

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Beryllium Sulfate, Beta ( $\beta$ -BeSO <sub>4</sub> )	CRYSTAL(β)	$M_r = 63.63583$	Beryllium Sulfate, Beta (BeSO <sub>4</sub> )	Be <sub>2</sub> O <sub>3</sub> S <sub>1</sub> (cr)
$\Delta_f H^\circ(298.15\text{ K}) = [79.258] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$				
$T_{m1} = 865\text{ K}$ ( $\alpha \rightarrow \beta$ )				
$T_{m2} = 908\text{ K}$ ( $\beta \rightarrow \gamma$ )				
<b>Enthalpy of Formation</b> The enthalpy of formation is calculated from that of the alpha phase by adding $\Delta_m H^\circ$ , since the heat capacities of both phases are assumed the same.				
<b>Heat Capacity and Entropy</b> The heat capacity was assumed to be the same as that of alpha phase. The entropy is calculated in a manner analogous to that used for the enthalpy of formation.				
<b>Transition Data</b> Refer to the $\alpha$ -crystal table for details.				
$\Delta_f H^\circ(298.15\text{ K}) = [-1199.695] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$				
$\Delta_m H^\circ = [-1199.695] \text{ J}\cdot\text{mol}^{-1}$				
$\Delta_m H^\circ = [1.113] \text{ kJ}\cdot\text{mol}^{-1}$				
$\Delta_m H^\circ = [19.552] \text{ kJ}\cdot\text{mol}^{-1}$				
0				
100				
200				
298.15	85.697	79.238	79.238	0.
300	86.111	79.789	79.259	0.159
400	103.880	107.156	82.870	9.714
500	116.357	131.743	90.231	20.756
600	126.817	153.878	99.024	32.913
700	137.988	174.253	108.332	46.145
800	149.787	193.446	117.782	60.531
900	162.046	211.792	127.215	76.120
1000	174.431	229.532	136.564	92.967
1100	183.088	246.583	145.797	110.864
1200	189.209	262.789	154.877	129.494
1300	193.543	278.114	163.773	148.643
1400	196.581	292.574	172.462	168.157
1500	198.656	306.211	180.928	187.925
1600	200.004	319.079	189.164	207.863
1700	200.706	331.228	197.167	227.903
1800	200.832	342.704	204.937	247.981
1900	200.832	353.563	212.476	268.065
2000	200.832	363.864	219.790	288.148
2100	200.832	373.663	226.886	308.231
2200	200.832	383.005	233.772	328.314
2300	200.832	391.933	240.456	348.397

CURRENT September 1966

PREVIOUS:

**Beryllium Sulfate, Gamma ( $\gamma$ -BeSO<sub>4</sub>)****CRYSTAL( $\gamma$ )****Be<sub>1</sub>O<sub>2</sub>S<sub>1</sub>(cr)**

$$\begin{aligned} S^\circ(298.15 \text{ K}) &= [100.784] \text{ J K}^{-1} \text{ mol}^{-1} \\ T_{\alpha\beta} &= 853 \text{ K } (\alpha \rightarrow \beta) \\ T_{\alpha\gamma} &= 908 \text{ K } (\beta \rightarrow \gamma) \end{aligned}$$

**Enthalpy of Formation**

The enthalpy of formation is calculated from that of the beta phase by adding  $\Delta_{\alpha\beta}H^\circ$ , since the heat capacities of both phases are assumed the same.

**Heat Capacity and Entropy**

The heat capacity was assumed to be the same as that of alpha phase. The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

**Transition Data**

Refer to the  $\alpha$ -crystal table for details.

$M_r = 105.06978$ Beryllium Sulfate, Gamma (BeSO <sub>4</sub> )	$\Delta_fH^\circ(0 \text{ K})$ Unknown	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$						Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$					
		$T/K$	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T)/T]$	$H^\circ - H^\circ(T_r)$	$\Delta_fH^\circ$	$\Delta_fG^\circ$	$T/K$	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T)/T]$	$H^\circ - H^\circ(T_r)$	$\Delta_fH^\circ$	$\Delta_fG^\circ$
0								200	85.697	100.784	100.784	0.	-1075.491
100								298.15	85.697	100.784	100.784	0.	-1070.143
200								300	86.111	101.316	100.786	0.159	-1070.166
300								400	101.380	128.682	104.396	9.714	-1074.841
400								500	116.357	153.270	111.757	20.756	-1039.523
500								600	126.817	175.405	120.550	32.913	-1034.098
600								700	137.988	195.780	129.859	46.145	-1034.113
700								800	149.787	214.973	139.309	60.531	-1031.128
800								900	162.046	233.319	148.742	76.120	-1081.123
900								1000	174.431	251.058	158.091	92.967	-1231.195
1000								1100	183.088	268.110	167.324	110.864	-1225.810
1100								1200	189.209	284.316	176.404	129.494	-1219.574
1200								1300	193.343	299.640	185.300	148.643	-1212.787
1300								1400	196.381	314.410	193.988	168.157	-1205.652
1400								1500	198.656	327.738	202.455	187.925	-1198.316
1500								1600	200.004	340.606	210.591	207.863	-1190.884
1600								1700	200.706	352.755	218.694	227.903	-1197.974
1700								1800	200.832	364.231	226.464	247.981	-1190.178
1800								1900	200.832	375.089	234.003	268.055	-1182.428
1900								2000	200.832	385.391	241.317	288.148	-1174.754
2000								2100	200.832	395.189	248.413	308.231	-1167.160
2100								2200	200.832	404.532	253.298	328.314	-1159.644
2200								2300	200.832	413.459	261.982	348.397	-1152.206
2300													-359.783
													-323.930
													-1144.843
													-1074.491

Beryllium Tungsten Oxide (BeWO<sub>4</sub>)

## CRYSTAL

$$S^\circ(298.15 \text{ K}) = [88.37 \pm 8.4] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$T_{hs} = \text{Unknown}$

## Enthalpy of Formation

The enthalpy of formation,  $\Delta_f H^\circ(\text{BeWO}_4, \text{cr}, 298.15 \text{ K}) = -361.7 \text{ kcal mol}^{-1}$ , is calculated from  $\Delta_f H^\circ(298.15 \text{ K}) = -17.1 \text{ kcal mol}^{-1}$  for  $\text{BeO(cr)} + \text{WO}_3(\text{cr}) \rightarrow \text{BeWO}_4(\text{cr})$ . The value of  $\Delta_f H^\circ(298.15 \text{ K})$  is assumed to be the same as that for  $\text{MgO(cr)} + \text{WO}_3(\text{cr}) \rightarrow \text{MgWO}_4(\text{cr})$ , using  $-143.7, -143.1, -201.5$ , and  $-362.3 \text{ kcal mol}^{-1}$  for the enthalpies of formation of  $\text{MgO(cr)}$ ,  $\text{BeO(cr)}$ ,  $\text{WO}_3(\text{cr})$  and  $\text{MgWO}_4(\text{cr})$ , respectively.

## Heat Capacity and Entropy

Heat capacities are estimated by comparison with those of  $\text{CaWO}_4(\text{cr})^1$ ,  $\text{BeO(cr)}^2$  and  $\text{CaO(cr)}^3$ . The entropy,  $S^\circ(298.15 \text{ K}) = 21.12 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ , is calculated from  $\Delta_f S^\circ(298.15 \text{ K}) = -0.4 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  for  $\text{BeO(cr)} + \text{WO}_3(\text{cr}) \rightarrow \text{BeWO}_4(\text{cr})$ . The value of  $\Delta_f S^\circ(298.15 \text{ K})$  is assumed to be the same as that for  $\text{MgO(cr)} + \text{WO}_3(\text{cr}) \rightarrow \text{MgWO}_4(\text{cr})$ , using 6.44, 3.38, 18.14 and 24.18  $\text{cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  for  $\text{MgO(cr)}$ ,  $\text{BeO(cr)}$ ,  $\text{WO}_3(\text{cr})$  and  $\text{MgWO}_4(\text{cr})$ , respectively.

## References

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- <sup>2</sup>JANAF Thermochemical Tables:  $\text{BeO}$  (cr), 9-30-65.
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$M_f = 256.85978$	Beryllium Tungsten Oxide (BeWO <sub>4</sub> )				Be <sub>1</sub> O <sub>4</sub> W <sub>1</sub> (cr)			
	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$	
	$\Delta_f H^\circ(\text{298.15 K}) = [-1513.4 \pm 63] \text{ kJ mol}^{-1}$	$\Delta_f H^\circ(\text{298.15 K}) = \text{Unknown}$	$C_p^\circ$	$S^\circ = -[G^\circ - H^\circ(T_r)]/T_r$	$H^\circ - H^\circ(T_r)/T_r$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0							$\log K_1$	
100								
200	97.278	88.366	88.366	0	-1513.353	-1404.818	246.118	
298.15	97.696	88.368	88.368	0.180	-1513.357	-1404.845	244.483	
300	97.698	92.397	92.397	0.1753	-1513.032	-1367.762	178.611	
400	112.968	119.279	100.491	22.600	-1511.920	-1331.561	139.107	
500	123.512	145.670						
600	131.336	168.909	109.980	35.357	-1510.306	-1295.634	112.795	
700	137.319	189.609	119.904	48.794	-1508.371	-1260.005	94.023	
800	142.884	208.312	129.804	62.806	-1506.174	-1224.671	79.963	
900	148.114	225.447	139.492	77.259	-1502.714	-1189.628	69.044	
1000	153.009	241.307	148.890	92.417	-1503.997	-1154.873	60.324	
1100	157.737	256.114	157.972	107.956	-1498.026	-1120.401	53.203	
1200	162.256	270.033	166.736	123.956	-1494.806	-1086.212	47.282	
1300	166.649	282.193	175.193	140.401	-1491.342	-1052.302	42.282	
1400	171.126	295.708	183.358	157.191	-1487.628	-1018.667	38.007	
1500	175.435	307.661	191.249	174.613	-1483.667	-985.307	34.311	
1600	179.912	319.126	198.885	192.386	-1491.988	-951.693	31.070	
1700	184.305	330.165	206.285	210.956	-1489.116	-917.947	28.205	
1800	188.698	340.824	213.465	222.247	-1483.922	-884.498	23.667	
1900	193.092	351.144	220.441	248.336	-1478.405	-851.345	23.405	
2000	197.485	361.160	227.238	267.865	-1472.565	-818.492	21.377	

PREVIOUS June 1963

CURRENT March 1967

Beryllium Tungsten Oxide (BeWO<sub>4</sub>)Be<sub>1</sub>O<sub>4</sub>W<sub>1</sub>(cr)

## NIST-JANAF THERMOCHEMICAL TABLES

## Beryllium Sulfide (BeS)

## CRYSTAL

 $M_r = 41.07218$  Beryllium Sulfide (BeS)

$$\Delta_f H^\circ(298.15 \text{ K}) = [37.03 \pm 4.2] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_m = 863 \text{ K}$$

## Enthalpy of Formation

Von Wartenberg<sup>1</sup> has measured the enthalpy of solution of Be and BeS in  $\text{H}_2\text{SO}_4$ . The difference between these two enthalpies gives  $\Delta_f H^\circ(333 \text{ K}) = -51.35 \pm 2.1 \text{ kcal}\cdot\text{mol}^{-1}$  for the reaction  $\text{Be}(\text{cr}) + \text{H}_2\text{S}(\text{g}) \rightarrow \text{BeS}(\text{cr}) + \text{H}_2(\text{g})$ . Using auxiliary JANAF<sup>2</sup> data we calculate  $\Delta_f H^\circ(\text{BeS, cr}, 298.15 \text{ K}) = -56.0 \pm 2.1 \text{ kcal}\cdot\text{mol}^{-1}$ . This is in agreement with the value for the enthalpy of formation preferred by NBS.<sup>3</sup>

## Heat Capacity and Entropy

No low-temperature heat capacity or high-temperature enthalpy measurements have been reported. We estimate  $C_p^\circ(298.15 \text{ K}) = 8.13 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  from the reaction  $\text{Be}(\text{cr}, \alpha) + \text{MgS}(\text{cr}) \rightarrow \text{BeS}(\text{cr})$  by assuming  $\Delta C_p^\circ = 0$ .<sup>2</sup> Comparison of this value with  $C_p^\circ$  data for all the alkaline earth oxides and sulfides<sup>2</sup> suggests that our estimate is reasonable.  $C_p^\circ$  data above 298.15 K are estimated graphically by comparison with  $\alpha$ - and  $\beta$ -BeO.<sup>2</sup>

Several methods of estimation predict that the value of  $S^\circ(298.15 \text{ K})$  should lie near 8.85 cal·K<sup>-1</sup>·mol<sup>-1</sup>. A graphical comparison of the standard entropies for other alkaline-earth oxides and sulfides suggests values for  $S^\circ(298.15 \text{ K})$  in the range 9–10 cal·K<sup>-1</sup>·mol<sup>-1</sup>, while additive entropy constants<sup>4</sup> give 6.8 (Kelly's)<sup>5</sup> and 9.3 (Lammer's) cal·K<sup>-1</sup>·mol<sup>-1</sup>. Literature estimates have included (in cal·K<sup>-1</sup>·mol<sup>-1</sup>) 7.4,<sup>6</sup> 8.0,<sup>6</sup> and 8.4.<sup>7</sup> We adopt  $S^\circ(298.15 \text{ K}) = 8.85 \pm 1.0 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  based on cation increments for a series of beryllium and magnesium compounds.

## Fusion Data

No literature melting data are available. BeO and BeS have a different crystal structure (cubic, zincblende type) than the remaining alkaline-earth oxides and sulfides (cubic, NaCl type).

## References

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- <sup>2</sup>JANAF Thermochemical Tables,  $\text{H}_2\text{S}(\text{g})$ , 6–30–77;  $\text{H}_2(\text{g})$ , 3–31–74;  $\text{MgO}(\text{cr})$ , 12–31–74;  $\text{SiO}(\text{cr})$ , 12–31–72;  $\text{CaO}(\text{cr})$ , 8–30–74;  $\text{BaO}(\text{cr})$ , 12–31–74;  $\text{Sr}(\text{cr})$ , 9–30–77.
- <sup>3</sup>U. S. Nat. Bur. Stand. Tech. Note 270–6, 119 pp. (1971).
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- <sup>5</sup>V. A. Kireev, Zh. Obshch. Khim., **16**, 1569 (1946).
- <sup>6</sup>P. J. Spencer, Atomic Energy Reviews No. 4 Beryllium, International Atomic Energy Agency, Vienna, (1973).
- <sup>7</sup>M. V. H. Karapetyants and M. L. Karapetyants, "Thermodynamic Constants of Inorganic and Organic Compounds," Eng. Trans. by J. Schmorak, Ann Arbor, (1970).

 $\text{Be}_1\text{S}_1(\text{cr})$ 

$T/K$	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T)]/T$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$			$\Delta_f H^\circ(T)$	$\log K_r$
			$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	Standard State Pressure = $p = 0.1 \text{ MPa}$		
0							
100							
200	34.016	37.028	0.			-234.304	-232.972
298.15	34.309	37.1240	0.063			-234.313	-232.964
300	400	48.151	33.932			-232.365	-203.444
400	500	47.698	38.483			-238.387	-231.067
500	600	51.045	41.475			-239.293	24.139
600	700	67.402	45.060			-239.509	19.981
700	800	55.145	82.694			-227.834	
900	900	56.651	89.278			-226.102	14.763
1000	1000	57.907	95.314			-223.264	12.958
1100	1100	58.968	100.883			-215.540	11.259
1200	1200	59.915	106.056			-207.937	9.874
1300	1300	60.762	110.886			-200.443	8.725
1400	1400	61.463	115.416			-193.049	7.757
1500	1500	61.955	119.673			-187.475	6.930
1600	1600	62.425	123.686			-178.523	6.217
1700	1700	62.839	127.484			-170.848	5.578
1800	1800	63.304	131.089			-162.834	5.003
1900	1900	63.769	134.525			-154.903	4.495
2000	2000	64.224	137.807			-147.050	4.043
2100	2100	64.664	140.951			-139.273	3.637
2200	2200	65.103	143.970			-131.639	3.273
2300	2300	65.542	146.873			-123.932	2.943
2400	2400	65.982	149.672			-116.363	2.643
2500	2500	66.421	152.374			-128.706	
2600	2600	66.860	154.988			-120.498	
2700	2700	67.300	157.520			-110.838	
2800	2800	67.739	159.975			-101.415	
2900	2900	68.178	162.360			-94.033	
3000	3000	68.618	164.679			-86.710	

<sup>1</sup>P. J. Spencer, Atomic Energy Reviews No. 4 Beryllium, International Atomic Energy Agency, Vienna, (1973).

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PREVIOUS

CURRENT September 1977

## Beryllium Sulfide (BeS)

## IDEAL GAS

## Beryllium Sulfide (BeS)

## Beryllium Sulfide (BeS)

$$S^{\circ}(298.15 \text{ K}) = 210.29 \pm 0.42 \text{ J K}^{-1} \text{mol}^{-1}$$

$$\Delta_f H^{\circ}(298.15 \text{ K}) = [261 \pm 63] \text{ kJ mol}^{-1}$$

$$\Delta_f H^{\circ}(0 \text{ K}) = [261 \pm 63] \text{ kJ mol}^{-1}$$

$$M_r = 41.07218$$

$$\Delta_f H^{\circ}(298.15 \text{ K}) = [261 \pm 63] \text{ kJ mol}^{-1}$$

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

$$C_p^* = \frac{S^* - [G^* - H^*(T_r)]/T}{J \cdot K^{-1} \cdot mol^{-1}}$$

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

$$H^* - H^*(T_r) / T = \frac{kJ \cdot mol^{-1}}{J \cdot K^{-1}}$$

$$\log K_r$$

Source	State	Electronic and Molecular Constants ( $\epsilon = 1$ )				
		$\epsilon_e, \text{cm}^{-1}$	$B_e, \text{Å}$	$r_e, \text{Å}$	$\alpha_e, \text{cm}^{-1}$	$\omega_e, \text{cm}^{-1}$
1, 2, 7	X <sup>+</sup> S <sup>-</sup>	0.0	1	1.7415	0.79559	0.0064
	[6600]	6	[1.9075]	[0.6590]	[702.46]	6.137
	A <sup>II</sup>	7842.9	2	1.9075	0.6590	762.46
	[A]	[13048.4]	2	[2.000]	[0.5997]	[61.6]
1, 2	S <sup>+</sup> A <sup>-</sup>	[21000]	3	[1.8137]	[0.72894]	[4.85]
	B <sup>1</sup> S <sup>+</sup>	25868.6	1	1.8137	0.72894	831.35
					0.0604	4.85

## Enthalpy of Formation

No experimental data are available on BeS(g). We estimate  $D^{\circ}_{\text{f}}(\text{BeS}, g)$  by the method of Hauge and Margrave<sup>1</sup> based on data involving known bond energies and force constants of the gaseous diatomic oxides and sulfides. Based on dissociation energies of the alkaline earth monoxides, taken from Srivastava,<sup>2</sup> dissociation energies of the alkaline earth sulfides and force constants calculated from JANAF data,<sup>3</sup> we calculate  $D^{\circ}_{\text{f}}(\text{BeS}, g) = 80 \pm 10 \text{ kcal mol}^{-1}$ . A normal linear-Birge-Sponer extrapolation of the ground state yields  $D^{\circ}_{\text{f}}(\text{BeS}, g) = 115 \text{ kcal mol}^{-1}$ . After correcting for ionic character<sup>4</sup> and for excited state products  $D^{\circ}_{\text{f}}(\text{BeS}, g) = 76 \text{ kcal mol}^{-1}$ . These values are very uncertain. See the discussion of MgS(e).<sup>5</sup> We adopt  $D^{\circ}_{\text{f}}(\text{BeS}, g) = 80 \pm 15 \text{ kcal mol}^{-1}$ . Using auxiliary JANAF data,<sup>3</sup> we calculate  $\Delta_f H^{\circ}(\text{BeS}, g, 298.15 \text{ K}) = 63 \pm 15 \text{ kcal mol}^{-1}$ .

## Heat Capacity and Entropy

The spectroscopic constants of the observed states taken from BeS(g).<sup>6</sup> 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 BeO<sup>7</sup> and from trends observed in the known states of the other alkaline-earth oxides and sulfides.<sup>3</sup> Uncertainty in the energy and molecular constants for the estimated states may contribute as much as 2–3 cal K<sup>-1</sup> mol<sup>-1</sup> to the entropy above 3000 K.

The splitting between the A<sup>1</sup>II and a<sup>1</sup>I states,  $\sim 1200 \text{ cm}^{-1}$ , is based on trends in the triplet-singlet splitting observed by Field<sup>8</sup> for the alkaline-earth oxides. The Hartree-Fock calculations of Verhaegen and Richards<sup>9</sup> support this. Their theoretical singlet-triplet splitting should be reasonably accurate even though the absolute energies are biased. The thermodynamic functions are calculated using first-order anharmonic corrections to Q<sub>1</sub> and Q<sub>2</sub> in the partition function Q = Q<sub>2</sub> Q<sub>1</sub> g exp (-ε<sub>eff</sub>/T).

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<sup>3</sup>JANAF Thermochanical Tables: Be(g), 9–30–71; S<sub>2</sub>(g), 12–31–65; BaO(g) and SrO(g), 6–30–74; BeO(g), MgO(g), and CaO(g), 12–31–74; MgS(g), CaS(g), SiS(g), and BaS(g), 9–30–77.

<sup>4</sup>C. J. Cheetah, W. J. M. Gisane, and R. F. Barrow, Trans. Faraday Soc. 61, 1308 (1965).

<sup>5</sup>B. Rosen, "Spectroscopic Data Relative to Diatomic Molecules," Pergamon Press, New York, (1970).

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<sup>8</sup>D. L. Hildenbrand, "Advances in High Temperature Chemistry," Vol. I, L. Eyring (ed.), pp. 198–206, Academic Press, New York, (1967).

<sup>9</sup>G. Verhaegen and W. G. Richards, Proc. Phys. Soc. (London) 90, 579 (1967).

<sup>10</sup>R. H. Hauge and J. L. Margrave, High Temp. Sci. 4, 170 (1972).

<sup>11</sup>R. D. Srivastava, High Temp. Sci. 8, 225 (1976).

<sup>12</sup>JANAF Thermochanical Tables: Be(g), 9–30–71; S<sub>2</sub>(g), 12–31–65; BaO(g) and SrO(g), 6–30–74; BeO(g), MgO(g), and CaO(g), 12–31–74; MgS(g), CaS(g), SiS(g), and BaS(g), 9–30–77.

<sup>13</sup>C. J. Cheetah, W. J. M. Gisane, and R. F. Barrow, Trans. Faraday Soc. 61, 1308 (1965).

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## Beryllium Sulfide (BeS)

CURRENT September 1977 (1 atm)

## Beryllium Sulfide (BeS)

PREVIOUS September 1977 (1 atm)

## NIST-JANAF THERMOCHEMICAL TABLES

**Be<sub>2</sub>(g)****M<sub>r</sub> = 18.02436 Beryllium (Be<sub>2</sub>)****IDEAL GAS**

$$D_0^* = 8.535 \pm 0.879 \text{ J·mol}^{-1}$$

$$S^*(298.15 \text{ K}) = 206.4 \pm 4.0 \text{ J·K}^{-1} \cdot \text{mol}^{-1}$$

$$\Delta H^{\circ}(0 \text{ K}) = 631.1 \pm 6.3 \text{ kJ·mol}^{-1}$$

$$\Delta H^{\circ}(298.15 \text{ K}) = 637.2 \pm 7.0 \text{ kJ·mol}^{-1}$$

		Spectroscopic Constants for Be <sub>2</sub> in cm <sup>-1</sup> (ground state)							
v	0	1	2	3	4	5	6	7	8
G(v)-G(0)	0	224	328.6	405.1	459.7	508	547.9	578.2	600.7
B(v)*	0.548	0.457	0.366	0.317	0.275	0.254	0.233	0.212	
10 <sup>a</sup> × D(v)*	10.13	10.13	10.13	31.64	31.64	31.64	31.64	31.64	

\*Estimated as explained below.

**Enthalpy of Formation**

The adopted value of the ground state dissociation energy for Be<sub>2</sub>(g),  $D_0^* = 8.535 \pm 0.879 \text{ kJ·mol}^{-1}$ , was determined via a high level quantum mechanical calculation by Lengsfeld, *et al.*<sup>1</sup> Using this value and the recommended value for  $\Delta_f H^{\circ}(\text{Be}_2, g, 0 \text{ K}) = 319.8 \text{ kJ·mol}^{-1}$  from CODATA,<sup>2</sup> we calculate the adopted value of  $\Delta_f H^{\circ}(\text{Be}_2, g, 0 \text{ K}) = 631.1 \pm 6.3 \text{ kJ·mol}^{-1}$ .

**Heat Capacity and Entropy**

The thermal functions were calculated using a direct summation technique analogous to the alkali dimers and diatomic halogens.<sup>12</sup> As in the diatomic fluorine case, the values of G(v), B<sub>v</sub>, and D<sub>v</sub> were directly input into the calculation. Values of 9 bound vibrational energy levels for the  $^1\Sigma^+$  ground state were determined from a high level *ab initio* quantum mechanical calculation (including full configuration interaction).<sup>3</sup> However, a recent spectroscopic determination by Bondybe<sup>4</sup> gave a value for  $\Delta G_{12\pi} = 224 \text{ cm}^{-1}$  which is 1.21 times larger than the corresponding value from the theoretical calculation. We therefore adopt  $\Delta G_{12\pi} = 224 \text{ cm}^{-1}$  and increase the rest of the theoretical energy determined vibrational spacings by the same factor. Since the theoretical binding energy of Harrison and Handy<sup>5</sup> may also be too small, we adopt the value calculated by Lengsfeld *et al.*<sup>1</sup> The adopted values of B<sub>v</sub> are estimated using the correlation of Calder and Ruedenberg<sup>6</sup>. Since a plot of  $\Delta G_{12\pi}$  vs. v exhibits two linear regions (0 ≤ v ≤ 3 and 4 ≤ v ≤ 8), the value of B<sub>v</sub> used to estimate  $\alpha_v$  in the 4 ≤ v ≤ 8 region is reduced from 0.593 to 0.39. This is done in order to assure a smoothly decreasing B<sub>v</sub> as v increases. The D<sub>v</sub> parameters are determined from the estimation method of Herzberg<sup>6</sup> where we use the first order D<sub>v</sub> term only.

The rotational levels are extrapolated to high J values according to the method of Khachkin<sup>7</sup> who proposed a simpler form of Wooley's method.<sup>8</sup> The rotational levels are weighed in accordance with the nuclear spin-rotation interaction<sup>9</sup> as follows: even J weight = 0.625, odd J weight = 0.375. The so-called quasibound rotational levels were not included in the calculation. No suitable spectroscopic information exists for any of the excited states of Be<sub>2</sub>. It should be noted that the inclusion of  $^3\Sigma^+$  and  $^3\Pi_g$  states in the range T ≥ 5000 K as proposed by Jones<sup>10</sup> would cause our calculated thermal functions to be deficient at temperatures greater than about 2000 K. Due to the extremely shallow well of the ground state, most Be<sub>2</sub> molecules will probably exist in an excited state at temperatures T ≥ 1000 K. The calculated S<sup>\*</sup>(298.15 K) is 5.41 J·K<sup>-1</sup>·mol<sup>-1</sup> smaller than the value adopted by Glushko, *et al.*<sup>11</sup>

**References**

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<sup>4</sup>V. E. Bondybe and J. H. English, *J. Chem. Phys.* **80**, 568 (1984).

<sup>5</sup>G. V. Calder and K. Ruedenberg, *J. Chem. Phys.* **49**, 5399 (1968).

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<sup>9</sup>Reference 6, Chapter 5.

<sup>10</sup>R. O. Jones, *J. Chem. Phys.* **71**, 1300 (1979).

<sup>11</sup>V. P. Glushko, V. Medvedev, *et al.*, "Thermal Constants of Substances," Volume IX, Moscow, (1979).

<sup>12</sup>JANAF Thermochemical Tables, *Li(g)*, 12-31-83; *F<sub>c</sub>(t)*, 6-30-82.

<sup>a</sup>See for example JANAF Thermochemical Tables, *Mg<sub>2</sub>(g)*, 9-30-83.

**Beryllium (Be<sub>2</sub>)**

		Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa	
		K <sup>-1</sup> ·mol <sup>-1</sup>	S <sup>*</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )/T]	K <sup>-1</sup> ·mol <sup>-1</sup>	A <sub>f</sub> H <sup>o</sup>
T/K	C <sub>v</sub>				
100	0	0	0	-9960	631.065
100	37.037	167.734	235.643	-67.911	631.065
100	346.091	194.091	209.116	-3.005	631.065
298.15	27.492	206.410	206.410	0	631.065
300	27.405	206.580	206.411	0.051	631.065
400	213.975	209.440	213.975	2.614	580.902
500	22.893	219.227	209.297	4.965	562.294
600	22.173	223.331	211.306	7.215	544.063
700	21.763	226.715	221.273	7.215	526.249
800	21.509	229.603	215.138	9.410	508.843
900	21.341	232.126	218.888	11.578	491.825
1000	21.226	234.368	218.576	13.714	475.175
1100	21.142	236.387	220.080	15.842	458.874
1200	21.081	238.224	221.498	20.071	442.906
1300	21.033	239.910	222.850	22.177	427.258
1400	20.997	241.467	224.125	24.278	405.414
1500	20.968	242.915	225.330	26.377	382.125
1600	20.944	244.267	226.472	28.472	368.707
1700	20.925	245.536	227.536	30.568	356.372
1800	20.909	246.732	228.589	32.657	344.256
1900	20.884	247.862	229.574	34.747	332.550
2000	20.851	248.933	230.515	36.836	320.644
2100	20.875	249.932	231.417	38.924	309.132
2200	20.866	250.923	232.281	41.011	297.805
2300	20.859	251.850	233.112	43.098	286.638
2400	20.853	252.738	233.912	53.012	275.685
2500	20.847	253.589	234.682	53.957	264.879
2600	20.843	254.407	235.425	49.353	528.858
2700	20.838	255.193	236.142	51.437	524.716
2800	20.834	255.951	236.836	53.521	513.384
2900	20.831	256.682	237.508	55.604	504.869
3000	20.828	257.388	238.159	57.687	495.485
3100	20.825	258.071	238.791	59.769	487.723
3200	20.823	258.732	239.403	61.816	479.116
3300	20.820	259.373	239.933	63.934	470.523
3400	20.818	259.994	240.578	66.016	463.722
3500	20.816	260.598	241.141	68.098	454.433
3600	20.815	261.184	241.650	70.179	445.432
3700	20.813	261.755	242.225	72.261	437.432
3800	20.812	262.310	242.746	74.342	393.040
3900	20.810	262.850	243.255	76.423	383.223
4000	20.809	263.377	243.759	78.504	372.023
4100	20.808	263.891	244.236	80.583	360.936
4200	20.807	264.392	244.710	82.666	350.856
4300	20.806	264.882	245.173	84.746	341.791
4400	20.805	265.360	245.627	86.827	329.962
4500	20.804	265.828	246.071	88.907	310.779
4600	20.803	266.285	246.505	90.988	301.628
4700	20.803	266.732	247.331	93.068	292.983
4800	20.802	267.170	247.348	95.148	284.536
4900	20.801	267.599	247.757	97.228	270.035
5000	20.801	268.019	248.188	99.348	260.364
5100	20.800	268.431	248.513	101.388	251.520
5200	20.799	268.835	248.927	103.458	242.797
5300	20.798	269.231	249.317	105.548	232.119
5400	20.798	269.620	249.689	107.623	225.556
5500	20.798	270.002	250.035	109.708	212.088
5600	20.798	270.377	250.414	111.788	197.911
5700	20.797	270.745	250.768	113.863	189.439
5800	20.797	271.106	251.115	115.947	183.259
5900	20.796	271.462	251.497	116.027	174.177
6000	20.796	271.811	251.794	121.191	165.972

CURRENT: September 1983 (1 bar)

**Be<sub>2</sub>(g)**

PREVIOUS:

**Beryllium Chloride ((BeCl<sub>2</sub>)<sub>2</sub>)****IDEAL GAS**

$$S^\circ(298.15\text{ K}) = [381.47]\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(298.15\text{ K}) = [-749]\text{ kJ}\cdot\text{mol}^{-1}$$

$$\text{Be}_2\text{Cl}_4(g)$$

$\nu, \text{cm}^{-1}$	$\nu, \text{cm}^{-1}$	Vibrational Frequencies and Degeneracies
100	0	0, 0, INFINITE
200	104.193	273.922
250	110.809	337.542
288.15	115.368	361.547
300	115.517	381.475
350	118.970	400.268
400	121.557	416.331
450	123.529	430.988
500	125.036	443.865
600	127.217	466.871
700	128.625	486.595
800	129.387	503.837
900	130.270	519.142
1000	130.771	532.894
1100	131.149	545.377
1200	131.440	556.801
1300	131.669	567.331
1400	131.832	577.096
1500	132.001	586.198
1600	132.123	594.721
1700	132.225	602.734
1800	132.311	610.295
1900	132.384	617.450
2000	132.446	624.242
2100	132.500	630.706
2200	132.546	636.871
2300	132.587	642.763
2400	132.623	648.407
2500	132.655	653.822
2600	132.683	659.025
2700	132.708	664.033
2800	132.731	668.860
2900	132.751	673.518
3000	132.769	678.019
3100	132.786	682.372
3200	132.801	686.588
3300	132.814	690.675
3400	132.827	694.640
3500	132.838	698.491
3600	132.849	702.233
3700	132.858	705.873
3800	132.867	709.416
3900	132.875	712.868
4000	132.883	716.232
4100	132.890	719.513
4200	132.897	722.715
4300	132.903	725.843
4400	132.909	728.898
4500	132.914	731.885
4600	132.919	734.806
4700	132.924	737.665
4800	132.928	740.464
4900	132.932	743.324
5000	132.936	745.890
5100	132.940	751.014
5200	132.943	751.104
5300	132.946	753.636
5400	132.950	756.122
5500	132.952	758.361
5600	132.955	760.957
5700	132.958	763.311
5800	132.960	765.622
5900	132.963	767.895
6000	132.965	770.130

**Enthalpy of Formation**  
The enthalpy of formation was estimated by assuming that the concentration of dimer in equilibrium with the monomer was  $-5\%$  at 500 K as reported by Hildenbrand, Theard, Murad and Ju,<sup>1</sup> giving an effective  $K_p = 5.5 \times 10^{-4}$  for  $2\text{BeCl}(g) \rightarrow \text{Be}_2\text{Cl}_4(g)$ .

**Heat Capacity and Entropy**  
The structure was assumed planar with a D<sub>2h</sub> symmetry, the bond lengths were estimated from the values for BeCl(g), a lengthening being assumed in the ring. The frequencies were estimated using K<sub>p</sub>Cl<sub>2</sub> as a basis for the ring vibrations. Two polymeric frequencies had been observed by Snelson.<sup>2</sup> These were observed in matrix isolated BeCl<sub>2</sub> gas and were ascribed to polymeric species on account of their warm up behavior. They are here assigned to the B<sub>3u</sub> asymmetric stretching mode and the B<sub>3u</sub> symmetric out of plane wag of the non-ring chlorines. The order of the frequencies listed above is arbitrary and not related to their species type. The principal moments of inertia are:  $I_x = [18.40488 \times 10^{-39}]$ ,  $I_y = [110.6214 \times 10^{-39}]$ , and  $I_z = [129.0303 \times 10^{-39}]$  g cm<sup>2</sup>.

**References**

- <sup>1</sup>D. L. Hildenbrand, L. P. Theard, E. Murad and F. Ju, Aeronutronic Div. of Philco Corp. Report U-3068, April 1965, under contract AF 04 (611)-8523.
- <sup>2</sup>A. Snelson, IIT Research Institute, Report No. IITRI-C 6013-4, May 1964, under contract No. DA-31-124-ARO (D)-111.

**M<sub>r</sub> = 159.83636 Beryllium Chloride ((BeCl<sub>2</sub>)<sub>2</sub>)**

<b>Enthalpy Reference Temperature = <math>T_r = 298.15\text{ K}</math></b>		<b>Standard State Pressure = <math>p = 0.1\text{ MPa}</math></b>	
$T/K$	$C_p^*$	$S^\circ - [G^\circ - H^\circ(T_r)/T]$	$H^\circ - H^\circ(T_r)$
0	0	0	-25.305
100	77.971	475.560	-752.015
200	104.193	391.721	-742.266
250	110.809	361.547	-750.678
288.15	115.368	381.475	-5.451
300	115.517	382.189	0
350	118.970	400.268	-748.936
400	121.557	416.331	-748.926
450	123.529	430.988	-747.650
500	125.036	443.865	-747.127
600	127.217	466.871	-744.001
700	128.625	486.595	-745.099
800	129.387	503.837	-745.159
900	130.270	519.142	-744.822
1000	130.771	532.894	-744.055
1100	131.149	545.377	-744.001
1200	131.440	556.801	-745.999
1300	131.669	567.331	-744.111
1400	131.832	577.096	-748.390
1500	132.001	586.198	-744.842
1600	132.123	594.721	-745.472
1700	132.225	602.734	-745.356
1800	132.311	610.295	-745.552
1900	132.384	617.450	-745.359
2000	132.446	624.242	-746.102
2100	132.500	630.706	-746.460
2200	132.546	636.871	-747.878
2300	132.587	642.763	-751.339
2400	132.623	648.407	-757.904
2500	132.655	653.822	-759.205
2600	132.683	659.025	-759.955
2700	132.708	664.033	-760.349
2800	132.731	668.860	-760.802
2900	132.751	673.518	-763.631
3000	132.769	678.019	-762.499
3100	132.786	682.372	-767.201
3200	132.801	686.588	-769.980
3300	132.814	690.675	-771.378
3400	132.827	694.640	-772.178
3500	132.838	698.491	-778.564
3600	132.849	702.233	-813.947
3700	132.858	705.873	-815.248
3800	132.867	709.416	-818.469
3900	132.875	712.868	-816.615
4000	132.883	716.232	-814.865
4100	132.890	719.513	-819.463
4200	132.897	722.715	-820.532
4300	132.903	725.843	-820.507
4400	132.909	728.898	-820.322
4500	132.914	731.885	-820.080
4600	132.919	734.806	-811.781
4700	132.924	737.665	-814.429
4800	132.928	740.464	-817.206
4900	132.932	743.324	-819.573
5000	132.936	745.890	-822.073
5100	132.940	748.523	-824.382
5200	132.943	751.104	-826.745
5300	132.946	753.636	-829.282
5400	132.950	756.122	-832.282
5500	132.952	758.361	-835.599
5600	132.955	760.957	-838.855
5700	132.958	763.311	-842.150
5800	132.960	765.622	-846.345
5900	132.963	767.895	-850.927
6000	132.965	770.130	-852.599

PREVIOUS: June 1965 (1 atm) CURRENT: June 1965 (1 bar)

**Beryllium Chloride ((BeCl<sub>2</sub>)<sub>2</sub>)**

$$\text{Be}_2\text{Cl}_4(g)$$

Beryllium Fluoride Oxide (O(BeF)<sub>2</sub>)

## IDEAL GAS

**M<sub>r</sub> = 72.020566 Beryllium Fluoride Oxide (O(BeF)<sub>2</sub>)**

$$S^{\circ}(298.15 \text{ K}) = [298.9] \text{ J K}^{-1} \cdot \text{mol}^{-1}$$

$$\Delta H^{\circ}(298.15 \text{ K}) = -1204.1 \pm 21 \text{ kJ mol}^{-1}$$

Vibrational Frequencies and Degeneracies	
v, cm <sup>-1</sup>	v, cm <sup>-1</sup>
0	0
100	231,587
200	270,625
250	285,913
298.15	76,151
300	76,314
350	80,365
400	83,817
450	86,772
500	89,304
600	93,336
700	96,312
800	98,534
900	100,216
1000	101,510
1100	102,521
1200	103,374
1300	103,969
1400	104,494
1500	104,927
1600	105,288
1700	105,591
1800	105,849
1900	106,059
2000	106,238
2100	106,422
2200	106,566
2300	106,691
2400	106,802
2500	106,901
2600	106,988
2700	107,066
2800	107,137
2900	107,200
3000	107,263
3100	107,309
3200	107,356
3300	107,399
3400	107,438
3500	107,475
3600	107,508
3700	107,538
3800	107,566
3900	107,593
4000	107,617
4200	107,660
4300	107,680
4400	107,698
4500	107,715
4600	107,731
4700	107,746
4800	107,760
4900	107,773
5000	107,785
5100	107,797
5200	107,808
5300	107,818
5400	107,828
5500	107,837
5600	107,846
5700	107,854
5800	107,862
5900	107,870
6000	107,877

σ = [2]

Ground State Quantum Weight: [1]  
 Point Group: [C<sub>2v</sub>]  
 Bond Distances: Be–O = [1.33] Å;  
 Bond Angles: O–Be–F = [180]°;  
 Product of the Moments of Inertia: I<sub>A</sub>/I<sub>C</sub> = [2.5549 × 10<sup>-14</sup>] g<sup>2</sup> cm<sup>6</sup>

## Enthalpy of Formation

Efimenco<sup>1</sup> has studied mass spectrometrically the reaction BeO(cr) + BeF<sub>2</sub>(g) → Be<sub>2</sub>OF<sub>2</sub>(g) and also reported two sets of equilibrium constants. Using JANAF thermal functions, the enthalpy of reaction has been calculated from those reported equilibrium constants by the 2nd law and the 3rd law methods.

Number of Measurements	T/K	ΔH°(298.15K), kcal·mol <sup>-1</sup>	Drift, cal·K <sup>-1</sup> ·mol <sup>-1</sup>
1st Set 13	1570–1891	41,448 ± 3.04	41,981
2nd Set 21*	1872–2195	42,553 ± 0.70	42,714

\*There are 4 points rejected due to failure of statistical test.

A weighted average value, ΔH°(298.15 K) = 42.70 kcal mol<sup>-1</sup>, was chosen for the enthalpy of reaction. The enthalpy of formation ΔH°(Be<sub>2</sub>OF<sub>2</sub>, g, 298.15 K) = 287.9 ± 5 kcal·mol<sup>-1</sup> and ΔH°(BeF<sub>2</sub>, g, 298.15 K) = 187.5 kcal·mol<sup>-1</sup>. The adopted “V” shape molecular structure with nine fundamental vibrational frequencies was obtained from an estimation by Mann.<sup>3</sup> The bond distance Be–O and Be–F were estimated to be the same as those in BeO(g) and BeF<sub>2</sub>(g), respectively. The principal moments of inertia are: I<sub>A</sub> = 1.0103 × 10<sup>-39</sup>, I<sub>B</sub> = 49.7842 × 10<sup>-39</sup>, and I<sub>C</sub> = 50.7946 × 10<sup>-39</sup> g·cm<sup>2</sup>.

## Heat Capacity and Entropy

The adopted “V” shape molecular structure with nine fundamental vibrational frequencies was obtained from an estimation by Mann.<sup>3</sup> The bond distance Be–O and Be–F were estimated to be the same as those in BeO(g) and BeF<sub>2</sub>(g), respectively. The principal moments of inertia are: I<sub>A</sub> = 1.0103 × 10<sup>-39</sup>, I<sub>B</sub> = 49.7842 × 10<sup>-39</sup>, and I<sub>C</sub> = 50.7946 × 10<sup>-39</sup> g·cm<sup>2</sup>.

## References

<sup>1</sup>J. Efimenco, NBS Report 8186, Ch. 13 (January, 1964), refer to pp. 103–112.

<sup>2</sup>D. E. Mann, NBS Report 8186, Ch. 15 (January, 1964); refer to pp. 118–121.

## IDEAL GAS

**M<sub>r</sub> = 72.020566 Beryllium Fluoride Oxide (O(BeF)<sub>2</sub>)**

Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa	
T/K	C°	S°	H° – H°(T <sub>r</sub> ) / T
0	0	0	INFINITE
100	47,638	231,587	-1204.127
200	65,525	305,569	-1204.705
250	71,486	300,144	-1204.493
298.15	76,151	298,915	0.
300	76,314	299,387	-1204.574
350	80,365	311,463	-1204.578
400	83,817	322,466	-1204.742
450	86,772	332,473	-1204.941
500	89,304	341,750	-1205,133
600	93,336	358,407	-1205,816
700	96,312	373,030	-1206,288
800	98,534	386,043	-1206,812
900	100,216	397,750	-1207,413
1000	101,510	408,378	-1208,448
1100	102,521	418,103	-1208,924
1200	103,374	427,059	-1209,867
1300	103,969	435,356	-1210,911
1400	104,494	443,080	-1212,190
1500	104,927	450,305	-1213,590
1600	105,288	457,089	-1244,232
1700	105,591	463,481	-1245,176
1800	105,849	469,524	-1246,160
1900	106,059	475,253	-1247,188
2000	106,238	480,699	-1248,259
2100	106,422	485,887	-1249,373
2200	106,566	490,841	-1249,827
2300	106,691	495,581	-1250,562
2400	106,802	500,124	-1251,723
2500	106,901	511,595	-1251,913
2600	106,988	516,224	-1252,956
2700	107,066	512,720	-1254,154
2800	107,137	516,615	-1255,582
2900	107,200	520,376	-1256,920
3000	107,263	526,041	-1257,372
3100	107,309	527,529	-1258,101
3200	107,356	532,926	-1258,906
3300	107,399	534,739	-1259,765
3400	107,438	537,447	-1260,630
3500	107,475	540,562	-1261,526
3600	107,508	543,590	-1262,430
3700	107,538	546,526	-1263,345
3800	107,566	549,564	-1264,260
3900	107,593	552,199	-1265,184
4000	107,617	554,923	-1266,493
4200	107,660	560,175	-1267,597
4300	107,680	562,708	-1268,696
4400	107,698	565,184	-1269,805
4500	107,715	567,160	-1270,914
4600	107,731	569,972	-1272,770
4700	107,746	572,289	-1274,514
4800	107,760	574,538	-1276,344
4900	107,773	576,780	-1278,597
5000	107,785	578,937	-1281,853
5100	107,797	581,092	-1282,513
5200	107,808	583,185	-1284,448
5300	107,818	585,239	-1286,531
5400	107,828	587,254	-1288,181
5500	107,837	589,233	-1290,000
5600	107,846	591,176	-1291,790
5700	107,854	593,085	-1293,550
5800	107,862	594,961	-1295,282
5900	107,870	596,805	-1296,988
6000	107,877	598,618	-1298,666

PREVIOUS: June 1966 (1 atm)

CURRENT: June 1966 (1 atm)

**Be<sub>2</sub>F<sub>2</sub>O<sub>1</sub>(g)****Be<sub>2</sub>F<sub>2</sub>O<sub>1</sub>(BeF)<sub>2</sub>**

## IDEAL GAS

 $\text{Be}_2\text{O(g)}$ Beryllium Oxide ( $\text{Be}_2\text{O}$ )M<sub>r</sub> = 34.02376 Beryllium Oxide ( $\text{Be}_2\text{O}$ )

$$S^{(298.15 \text{ K})} = [220.8] J \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$\Delta H^{\circ}(0 \text{ K}) = -64 \pm 42 \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta H^{\circ}(298.15 \text{ K}) = -63 \pm 42 \text{ kJ} \cdot \text{mol}^{-1}$$

Vibrational Frequencies and Degeneracies		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$				Standard State Pressure = $p^* = 0.1 \text{ MPa}$			
$\nu, \text{cm}^{-1}$	$\sigma = 2$	$T \text{ K}$	$C^*$	$S^*$	$-(G^* - H^*(T)) / T$	$H^* - H^*(T) / T$	$\Delta H^*$	$\Delta G^*$	
0	0	0	0	0	INFINITE	-9.925	-64.479	-64.479	
100	29.748	183.340	253.419	-7.008	-63.092	-72.660	-37.954	-INFINITE	
200	35.536	205.584	224.408	-3.765	-62.460	-82.559	21.562		
250	38.466	213.835	221.488	-1.913	-62.521	-87.581	18.299		
298.15	40.952	220.827	220.827	0.	-62.760	-92.388	16.186		
300	41.041	221.081	220.828	0.076	-62.772	-92.572	16.118		
350	43.322	227.582	221.336	2.181	-63.156	-97.510	14.553		
400	45.354	233.502	222.492	4.046	-63.914	-102.387	13.370		
450	47.163	238.551	224.022	6.718	-64.112	-107.204	12.444		
500	48.767	244.004	225.771	9.117	-64.636	-111.964	11.697		
600	51.429	253.141	229.588	14.132	-65.734	-121.327	10.562		
700	53.482	261.230	233.541	19.382	-66.994	-130.502	9.738		
800	55.063	268.480	237.463	65.448	-68.125	-139.506	9.109		
900	56.290	273.039	241.860	30.383	-69.443	-148.350	8.610		
1000	57.240	281.051	244.939	36.062	-70.361	-157.043	8.203		
1100	58.011	286.515	248.491	41.826	-72.394	-165.598	7.863		
1200	58.620	291.590	251.874	47.659	-74.052	-173.988	7.573		
1300	59.115	296.502	255.112	53.547	-75.846	-182.244	7.323		
1400	59.520	300.698	258.213	59.479	-77.785	-190.357	7.102		
1500	59.836	304.816	261.184	65.448	-79.877	-198.376	6.906		
1600	60.138	309.689	264.033	71.449	-111.202	-205.098	6.696		
1700	60.375	312.342	268.769	74.744	-112.818	-210.917	6.481		
1800	60.577	315.799	269.397	83.522	-114.467	-216.641	6.287		
1900	60.750	319.079	271.926	88.389	-116.153	-222.271	6.111		
2000	60.899	322.198	274.363	95.671	-117.877	-227.812	5.950		
2100	61.029	325.015	276.712	101.788	-119.641	-233.265	5.802		
2200	61.142	328.015	278.980	107.877	-121.448	-243.634	5.666		
2300	61.242	330.735	281.171	113.996	-123.298	-243.919	5.540		
2400	61.330	333.343	283.291	120.125	-125.193	-249.121	5.422		
2500	61.408	335.848	285.344	126.262	-127.134	-254.247	5.312		
2600	61.478	338.258	287.333	132.406	-129.121	-259.293	5.209		
2700	61.540	340.580	289.662	138.557	-131.155	-264.261	5.112		
2800	61.596	342.819	291.133	144.714	-131.555	-267.077	5.012		
2900	61.647	344.981	292.935	150.376	-131.526	-270.335	4.929		
3000	61.692	347.072	294.724	157.043	-131.516	-273.961	3.900		
3100	61.734	349.095	296.446	163.214	-131.503	-277.587	3.498		
3200	61.771	351.107	298.122	169.390	-131.528	-191.212	3.121		
3300	61.806	352.937	299.733	175.569	-171.533	-174.834	2.767		
3400	61.837	354.803	301.347	181.751	-175.441	-188.454	2.434		
3500	61.866	356.395	311.493	187.936	-175.576	-142.070	2.120		

## Enthalpy of Formation

Hildenbrand, Theard, and Ju<sup>1</sup> have reported the enthalpy of formation. Equilibrium constants were determined in a mass spectrometer for the reactions  $2\text{BeO(cr)} \rightarrow \text{Be}_2\text{O(g)} + \text{O(g)} - (1)$ ;  $\text{Be}_2\text{O(g)} + \text{O(g)} \rightarrow \text{Be}_2\text{O}_2\text{g}$  — (2); and  $\text{Be}_2\text{O}_2\text{g} \rightarrow \text{Be}_2\text{O(g)} + \text{O(g)} - (3)$ . Using our own Gibbs energy functions we obtain  $\Delta_f H^{\circ}$ ( $\text{Be}_2\text{O}$ , g, 298.15 K) = 13.1, — 14.5, and — 16.7 kcal·mol<sup>-1</sup>, all ± 10%; the 2nd law treatment of reaction 1 gives — 18.3 ± 10 kcal·mol<sup>-1</sup>. We adopt a median value — 15 ± 10 kcal·mol<sup>-1</sup>.

## Heat Capacity and Entropy

Buchlier, Stauffer, Klempner and Wharton<sup>2</sup> have shown  $\text{Li}_2\text{O}$  to be linear. Also Walsh<sup>1</sup> predicted that  $\text{AB}_2$  molecules with less than 16 bonding electrons would be linear. Thus  $\text{Be}_2\text{O}$  was taken to be linear and symmetrical, with a Be—O bond length of 1.4 Å, which is a little longer than in  $\text{BeO(g)}$ .<sup>3</sup> The vibrational frequencies were estimated by taking  $v_1$  to be larger than the stretch in  $\text{BeO(g)}$  and then calculating  $v_1$  from the valence force field assumption. The bending force constant was estimated as 1/20th of the stretching force constant. The two outermost electrons were considered unpaired and so gave a  $\Sigma$  ground state.

## References

- <sup>1</sup>D. L. Hildenbrand, L. P. Theard, and F. Ju, Ford Motor Co., Aerotronic Division, Third Quarterly Technical Report U-2231, (April-June 1963).
- <sup>2</sup>A. Buchler, J. L. Stauffer, W. Klempner and C. Wharton, A. D. Little, Inc., Interim Technical Report No. 5, (1963).
- <sup>3</sup>A. D. Walsh, J. Chem. Soc. London 1953, 2269.

 $\text{Be}_2\text{O}_2\text{(g)}$ 

$S^{(298.15 \text{ K})} = [220.8] J \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$	$\Delta H^{\circ}(0 \text{ K}) = -64 \pm 42 \text{ kJ} \cdot \text{mol}^{-1}$	$\Delta H^{\circ}(298.15 \text{ K}) = -63 \pm 42 \text{ kJ} \cdot \text{mol}^{-1}$	$T \text{ K}$	$C^*$	$S^*$	$-(G^* - H^*(T)) / T$	$H^* - H^*(T) / T$	$\Delta H^*$	$\Delta G^*$	$\log K_r$
0	0	0	0	0	0	INFINITE	-9.925	-64.479	-64.479	-INFINITE
100	29.748	183.340	253.419	-7.008	-63.092	-72.660	-37.954			
200	35.536	205.584	224.408	-3.765	-62.460	-82.559	21.562			
250	38.466	213.835	221.488	-1.913	-62.521	-87.581	18.299			
298.15	40.952	220.827	220.827	0.	-62.760	-92.388	16.186			
300	41.041	221.081	220.828	0.076	-62.772	-92.572	16.118			
350	43.322	227.582	221.336	2.181	-63.156	-97.510	14.553			
400	45.354	233.502	222.492	4.046	-63.914	-102.387	13.370			
450	47.163	238.551	224.022	6.718	-64.112	-107.204	12.444			
500	48.767	244.004	225.771	9.117	-64.636	-111.964	11.697			
600	51.429	253.141	229.588	14.132	-65.734	-121.327	10.562			
700	53.482	261.230	233.541	19.382	-66.994	-130.502	9.738			
800	55.063	268.480	237.463	65.448	-68.125	-139.506	9.109			
900	56.290	273.039	241.860	30.383	-69.443	-148.350	8.610			
1000	57.240	281.051	244.939	36.062	-70.361	-157.043	8.203			
1100	58.011	286.515	248.491	41.826	-72.394	-165.598	7.863			
1200	58.620	291.590	251.874	47.659	-74.052	-173.988	7.573			
1300	59.115	296.502	255.112	53.547	-75.846	-182.244	7.323			
1400	59.520	300.698	258.213	59.479	-77.785	-190.357	7.102			
1500	59.836	304.816	261.184	65.448	-79.877	-198.376	6.906			
1600	60.138	309.689	264.033	71.449	-111.202	-205.098	6.696			
1700	60.375	312.342	268.769	74.744	-112.818	-210.917	6.481			
1800	60.577	315.799	269.397	83.522	-114.467	-216.641	6.287			
1900	60.750	319.079	271.926	88.389	-116.153	-222.271	6.111			
2000	60.899	322.198	274.363	95.671	-117.877	-227.812	5.950			
2100	61.029	325.015	276.712	101.788	-119.641	-233.265	5.802			
2200	61.142	328.015	278.980	107.877	-121.448	-243.634	5.666			
2300	61.242	330.735	281.171	113.996	-123.298	-243.919	5.540			
2400	61.330	333.343	283.291	120.125	-125.193	-249.121	5.422			
2500	61.408	335.848	285.344	126.262	-127.134	-254.247	5.312			
2600	61.478	338.258	287.333	132.406	-129.121	-259.293	5.209			
2700	61.540	340.580	289.662	138.557	-131.155	-264.261	5.112			
2800	61.596	342.819	291.133	144.714	-131.555	-267.077	4.929			
2900	61.647	344.981	292.935	150.376	-131.526	-270.335	4.829			
3000	61.692	347.072	294.724	157.043	-131.516	-273.961	3.900			
3100	61.734	349.095	296.446	163.214	-131.503	-277.587	3.498			
3200	61.771	351.107	298.122	169.390	-131.528	-191.212	3.121			
3300	61.806	352.937	299.733	175.569	-171.533	-174.834	2.767			
3400	61.837	354.803	301.347	181.751	-175.441	-188.454	2.434			
3500	61.866	356.395	311.493	187.936	-175.576	-142.070	2.120			
3600	61.893	358.339	304.416	194.124	-175.622	-125.682	1.843			
3700	61.917	360.339	305.896	200.314	-175.953	-109.288	1.543			
3800	61.940	361.687	307.343	206.507	-176.277	-86.888	1.243			
3900	61.961	363.296	308.157	212.702	-176.989	-76.481	1.024			
4000	61.980	364.865	310.140	218.899	-176.845	-60.067	0.784			
4100	61.998	367.095	312.818	231.299	-177.246	-43.642	0.556			
4200	62.015	367.475	321.397	237.510	-178.230	-27.208	0.338			
4300	62.030	369.349	314.116							

## NIST-JANAF THERMOCHEMICAL TABLES

 $\text{Be}_2\text{O}_2(\text{g})$  $M_r = 50.02316$  Beryllium Oxide ((BeO)<sub>2</sub>)

## IDEAL GAS

$$S^\circ(298.15 \text{ K}) = [247.61] \text{ J K}^{-1} \cdot \text{mol}^{-1}$$

$$\Delta H^\circ(0 \text{ K}) = -409 \pm 50 \text{ kJ mol}^{-1}$$

$$\Delta H^\circ(298.15 \text{ K}) = -410 \pm 50 \text{ kJ mol}^{-1}$$

$T/K$	$C_p^*$	$S^\circ - [G^\circ - H^\circ(T,)]/T$	$H^\circ - H^\circ(T,)/T$	$\Delta_H^\circ$	$\Delta_G^\circ$	$\log K_r$
0	0.	INFINITE	-11.409	-408.893	-408.893	INFINITE
100	33.845	204.646	-8.075	-408.575	-411.555	108.265
200	40.459	259.794	251.839	-449.7	-408.942	86.893
250	45.019	239.309	248.400	-227.5	-409.438	-415.877
298.15	49.339	247.611	247.611	0.	-410.032	-417.064
300	49.499	247.917	247.612	0.091	-410.056	-417.107
350	53.618	255.862	248.230	2.671	-418.231	-421.418
400	57.274	263.266	249.622	5.445	-411.357	-419.261
450	60.436	270.200	251.554	8.391	-420.211	-48.777
500	63.197	276.715	253.748	11.484	-412.583	-421.093
600	67.555	288.643	258.589	18.033	-413.728	-422.687
700	70.753	299.510	263.658	24.956	-414.842	-424.092
800	73.124	308.920	268.725	32.156	-415.973	-425.337
900	74.910	317.641	273.683	39.561	-417.157	-426.437
1000	76.277	325.607	278.433	47.124	-418.423	-427.401
1100	77.342	332.929	283.105	54.807	-419.791	-428.233
1200	78.185	339.696	287.542	62.526	-420.128	-428.936
1300	78.861	345.982	291.799	70.438	-422.898	-429.510
1400	79.410	351.847	295.881	78.353	-424.662	-430.042
1500	79.863	357.342	299.797	86.317	-426.580	-430.265
1600	80.229	362.508	303.556	94.323	-457.732	-429.393
1700	80.555	367.382	307.169	102.363	-459.180	-427.577
1800	80.823	371.994	310.643	110.432	-460.666	-425.676
1900	81.051	376.371	313.988	118.526	-462.194	-423.690
2000	81.248	380.533	317.712	126.641	-463.767	-421.623
2100	81.419	384.501	320.523	134.775	-465.387	-419.476
2200	81.568	388.293	323.327	142.924	-467.057	-417.251
2300	81.692	391.921	326.231	151.083	-468.778	-414.949
2400	81.813	395.401	329.041	159.263	-470.553	-412.761
2500	81.915	398.743	331.765	167.450	-472.382	-410.118
2600	82.006	401.957	334.401	175.646	-474.265	-407.590
2700	82.087	405.054	336.961	183.851	-476.204	-404.989
2800	82.160	408.041	339.446	192.063	-480.112	-389.869
2900	82.226	410.926	340.862	200.283	-486.036	-365.924
3000	82.285	413.713	344.211	208.508	-492.000	-342.000
3100	82.339	416.412	346.496	216.440	-495.955	-318.068
3200	82.388	419.027	348.722	224.976	-497.955	-294.137
3300	82.432	421.563	350.891	233.217	-503.987	-270.205
3400	82.473	424.025	353.006	241.462	-506.053	-246.270
3500	82.510	426.416	355.070	249.711	-506.156	-222.335
3600	82.545	428.741	357.084	257.964	-506.300	-198.395
3700	82.576	431.003	359.098	266.220	-506.489	-174.451
3800	82.605	433.231	361.974	274.479	-506.726	-150.543
3900	82.632	435.351	362.854	282.741	-507.016	-126.543
4000	82.657	437.444	364.692	291.006	-506.363	-102.578
4100	82.681	439.485	366.492	299.273	-506.171	-78.604
4200	82.702	441.478	368.234	307.542	-506.242	-54.618
4300	82.722	443.424	369.979	315.813	-506.784	-30.621
4400	82.741	445.326	371.670	323.086	-506.399	-13.781
4500	82.759	447.186	373.328	332.961	-506.091	-17.415
4600	82.775	449.005	374.933	340.638	-506.864	-4.801
4700	82.791	450.785	376.548	348.916	-507.723	-1.340
4800	82.805	452.528	378.113	357.196	-506.670	-0.975
4900	82.819	454.236	379.649	365.477	-507.210	-0.372
5000	82.832	455.909	381.157	373.760	-508.384	-0.078
5100	82.844	457.550	382.639	382.044	-507.081	-1.659
5200	82.855	459.158	384.095	390.329	-507.418	-1.870
5300	82.866	460.737	385.526	398.615	-507.860	-2.073
5400	82.876	462.286	386.934	405.902	-512.555	-2.269
5500	82.886	463.807	388.318	415.190	-507.606	-2.458
5600	82.895	465.300	389.679	423.479	-507.836	-2.641
5700	82.903	466.767	391.019	431.769	-507.097	-2.817
5800	82.912	468.209	392.337	440.060	-508.715	-2.988
5900	82.919	469.627	393.635	448.351	-508.328	-3.155
6000	82.927	471.020	394.913	456.643	-508.057	-3.313

Enthalpy of Formation  
Chupka, Berkowitz, and Giese<sup>1</sup> studied the temperature dependence of the type 2A<sub>1g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, and B<sub>3g</sub>. These were estimated by comparison with (LiO)<sub>2</sub> for which values have been calculated by White, Seshadri, Dever, Mann, and Linnevsky.<sup>2</sup> It seems unlikely that any other structure than that of a ring is possible, as, in order to approach the observed equilibrium constant an even lower entropy is needed. A non-linear chain would have a higher entropy due to the change in symmetry number and the two odd electrons. A linear chain would have approximately the same entropy due to cancellation of opposite effects. The vibrational frequencies were also made as high as possible by normalizing them using B<sub>w</sub> equal to the BeO stretch in BeO(g). The bond length was taken as the sum of the covalent radii of O and Be, which is in general agreement with other polymeric structures which generally increase in bond length by 10–20% in going from monomer to polymer. The bond angle was chosen arbitrarily; however, changes in the angle would change the entropy less than 1 cal K<sup>-1</sup> mol<sup>-1</sup>.

The principal moments of inertia are: I<sub>A</sub> = 7.0589 × 10<sup>-39</sup>, I<sub>B</sub> = 3.9761 × 10<sup>-39</sup>, and I<sub>C</sub> = 11.0350 × 10<sup>-39</sup> g cm<sup>2</sup>.  
<sup>1</sup>W. A. Chupka, J. Berkowitz and C. F. Giese, J. Chem. Phys., 30, 827 (1959).  
<sup>2</sup>D. White, K. Seshadri, D. F. Dever, D. E. Mann, and M. J. Linnevsky, prepublication communication, (July 1963).

## References

- 1W. A. Chupka, J. Berkowitz and C. F. Giese, J. Chem. Phys., 30, 827 (1959).
- 2D. White, K. Seshadri, D. F. Dever, D. E. Mann, and M. J. Linnevsky, prepublication communication, (July 1963).

CURRENT September 1963 (1 atm)

Beryllium Oxide ((BeO)<sub>2</sub>)  
Beryllium Oxide ((BeO)<sub>2</sub>)  
PREVIOUS September 1963 (1 atm)

Beryllium Silicate ( $\text{Be}_2\text{SiO}_4$ )

## CRYSTAL

$$\Delta H^\circ(0 \text{ K}) = [-2105 \pm 29] \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta H^\circ(298.15 \text{ K}) = [-2117 \pm 29] \text{ kJ} \cdot \text{mol}^{-1}$$

	$T_{\text{fus}} = 1833 \text{ K}$	$\text{Be}_2\text{O}_3(\text{cr})$
Enthalpy of Formation		

The  $\Delta_fH^\circ(298.15 \text{ K})$  was estimated from the  $\Delta_fH^\circ(298.15 \text{ K})$  of Mg, Ca and Ba oxides with  $\text{SiO}_2$  given by Kelley<sup>1</sup> and from the  $\Delta_fH^\circ(298.15 \text{ K})$  of  $\text{BeO}(\text{cr})$  and  $\text{SiO}_2(\text{cr})$  in the JANAF tables.<sup>2</sup> The  $\Delta_fH^\circ(298.15 \text{ K}) = 0 \pm 7 \text{ kcal} \cdot \text{mol}^{-1}$  was estimated for the reaction  $2\text{BeO}(\text{cr}) + \text{SiO}_2(\text{cr}) \rightarrow \text{Be}_2\text{SiO}_4(\text{cr})$ .

## Heat Capacity and Entropy

At low temperatures  $C_p$  was used from Kelley.<sup>4</sup> Above 298.15 K,  $C_p$  values were estimated by summation of the component oxides using the JANAF tables,<sup>2</sup>  $\text{BeO}$  and  $\text{SiO}_2$ . The entropy was calculated at 34.7 K using the Debye and Planck-Einstein functions  $D(32/T) + 2E(32/T)$  given by Kelley.<sup>4</sup> The value of  $S^\circ(54.7 \text{ K}) = 13.59 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ .

## Fusion Data

The incongruent melting point was taken from Kubaschewski and Evans.<sup>4</sup>

## References

- <sup>1</sup>K. K. Kelley, U.S. Bur. Mines, RI-5901, 32, pp. (1962).
- <sup>2</sup>JANAF Thermochemical Table,  $\text{BeO}(\text{cr})$ , 9-30-63,  $\text{SiO}_2(\text{cr})$ , 12-30-62.
- <sup>3</sup>K. K. Kelley, J. Am. Chem. Soc., 61, 1217 (1939).
- <sup>4</sup>O. Kubaschewski and E. L. Evans, "Metallurgical Thermochemistry" 3rd. edition, Pergamon Press, New York, 426 pp. (1959).

		Beryllium Silicate ( $\text{Be}_2\text{SiO}_4$ )				Beryllium Silicate ( $\text{Be}_2\text{SiO}_4$ )			
		Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$				Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$			
		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		$H^\circ - H^\circ(T_r)$		$\Delta H^\circ$		$\Delta G^\circ$	
		$T/\text{K}$	$C_p^\circ$	$J \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$	$S^\circ$	$-[G^\circ - H^\circ(T)]/T$	$\text{kJ} \cdot \text{mol}^{-1}$	$\text{kJ} \cdot \text{mol}^{-1}$	$\log K_r$
0	0	0	0.794	0	0	INFINITE	-12.227	-2105.003	INFINITE
100	100	18.794	7.470	124.264	-11.679	-2110.509	-2076.211	-1044.501	
200	200	60.433	33.245	71.847	-7.720	-2114.806	-2040.059	-532.809	
298.15	298.15	95.563	64.190	64.190	0	-2117.225	-2002.794	350.881	
300	300	96.098	64.782	64.191	0.177	-2117.255	-2002.084	348.594	
400	400	120.750	96.007	68.281	11.090	-2118.090	-1963.528	256.411	
500	500	136.942	124.764	76.748	24.008	-2117.773	-1924.506	201.094	
600	600	149.160	150.850	86.960	38.324	-2116.676	-1886.125	164.228	
700	700	158.866	174.605	97.810	53.577	-2114.993	-1848.175	137.913	
800	800	166.021	196.312	108.786	70.021	-2112.905	-1810.198	118.194	
900	900	170.749	216.154	119.630	86.872	-2110.613	-1772.996	102.873	
1000	1000	174.054	234.324	130.204	104.120	-2108.265	-1735.053	90.630	
1100	1100	176.556	251.025	140.439	121.644	-2105.957	-1697.844	80.624	
1200	1200	178.197	266.451	150.305	139.375	-2103.739	-1660.841	72.295	
1300	1300	179.636	280.773	159.797	157.268	-2101.643	-1624.019	65.254	
1400	1400	180.916	294.134	168.921	175.298	-2099.687	-1587.353	59.225	
1500	1500	181.387	306.649	177.690	193.439	-2097.894	-1550.822	54.004	
1600	1600	182.849	318.418	186.121	211.676	-2095.553	-1513.553		
1700	1700	183.803	329.532	194.233	230.008	-2125.349	-1474.725	49.406	
1800	1800	184.749	340.065	202.045	248.436	-2173.281	-1433.704	45.313	
1900	1900	185.686	350.079	209.575	266.958	-2168.403	-1392.819	41.605	
2000	2000	186.606	359.627	216.841	285.572	-2165.938	-1352.061	35.312	
2100	2100	187.493	368.753	223.859	304.277	-2163.512	-1311.427	32.620	
2200	2200	188.380	377.496	230.645	323.071	-2161.066	-1270.907	30.175	
2300	2300	189.267	385.889	237.213	341.954	-2158.618	-1230.501		
2400	2400	190.154	393.963	243.578	360.925	-2156.170	-1190.202	25.904	
2500	2500	191.041	401.743	249.750	379.984	-2153.720	-1150.003	24.028	
2600	2600	191.928	409.253	255.741	399.133	-2151.267	-1109.903	22.298	
2700	2700	192.815	416.513	261.562	418.370	-2148.810	-1069.896	20.693	
2800	2800	193.702	423.542	267.222	437.696	-2148.262	-1017.536	18.982	
2900	2900	194.589	430.354	272.730	457.111	-2143.668	-956.521	17.229	
3000	3000	195.476	436.966	278.095	476.614	-2149.034	-895.663	15.595	

Beryllium Silicate ( $\text{Be}_2\text{SiO}_4$ ) $\text{Be}_2\text{O}_3\text{Si}_1(\text{cr})$ 

PREVIOUS: September 1961

CURRENT: June 1965

## Beryllium Nitride, Alpha ( $\alpha$ -Be<sub>3</sub>N<sub>2</sub>) CRYSTAL( $\alpha$ )

$$M_r = 5.04994 \text{ Beryllium Nitride, Alpha (Be}_3\text{N}_2)$$

$$\Delta_f H^\circ(0 \text{ K}) = -580.9 \pm 1.3 \text{ kJ/mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = -588.3 \pm 1.3 \text{ kJ/mol}^{-1}$$

$$\Delta_{\text{fus}}H^\circ = [129.3] \text{ kJ}\cdot\text{mol}^{-1}$$

## Enthalpy of Formation

Gross, Hayman, Greene and Bingham<sup>1</sup> have measured the enthalpy of Chlorination of  $\alpha$ -Be<sub>2</sub>N<sub>2</sub> to  $\alpha$ -BeCl<sub>2</sub>, and the enthalpy of reaction of Be with ammonia. The chlorination reaction (A)  $\alpha$ -Be<sub>2</sub>N<sub>2</sub>(cr) + 3Cl<sub>2</sub>(g)  $\rightarrow$  3  $\alpha$ -BeCl<sub>2</sub>(cr) + N<sub>2</sub>(g) had a  $\Delta H_f^{\circ}$ (298.15 K) = -210.3  $\pm$  0.4 kcal mol<sup>-1</sup> which, combined with the value of -117.1  $\pm$  0.4 kcal mol<sup>-1</sup> for  $\alpha$ -BeCl<sub>2</sub> reported in the same paper, yields  $\Delta H_f^{\circ}$ ( $\alpha$ -Be<sub>2</sub>N<sub>2</sub>, cr, 298.15 K) = -141.0  $\pm$  1.6 kcal mol<sup>-1</sup>. Reaction (B) 3BeCl<sub>2</sub> + 2 NH<sub>3</sub>(g)  $\rightarrow$   $\alpha$ -Be<sub>2</sub>N<sub>2</sub>(cr) + 3 HCl(g) had a  $\Delta H_f^{\circ}$ (298.15 K) = -214.6  $\pm$  0.3 kcal mol<sup>-1</sup>, which, combined with the JANAF<sup>2</sup> value for NH<sub>3</sub>(g), yields  $\Delta H_f^{\circ}$ ( $\alpha$ -Be<sub>2</sub>N<sub>2</sub>, cr, 298.15 K) = -140.3  $\pm$  0.3 kcal mol<sup>-1</sup>. A weighted mean value of the above two determinations is adopted.

Source	T/K	Points	$\Delta H^\circ(298.15\text{ K})$	kcal·mol <sup>-1</sup>	Drift cal·K <sup>-1</sup> ·mol <sup>-1</sup>	$\Delta H^\circ(298.15\text{ K})$ kcal mol <sup>-1</sup>
1	1478-1592	9*	364.5 ± 5.9	374.00	6.0 ± 3.8	-139.23
1	1541-1652	15*	369.6 ± 8.3	376.51	4.0 ± 5.3	-141.74
1	1438-1661	14	347.7 ± 3.7	374.54	16.9 ± 2.4	-139.77
1	1450-1646	17*	366.7 ± 8.9	375.28	4.8 ± 5.7	-140.51
3	1473-1611	52*	358.9 ± 5.1	375.41	10.3 ± 3.3	-140.64
4	1767-1946	14	355.8 ± 3.3	377.77	11.9 ± 1.8	-143.00
4	1660-1891	10	395.0 ± 5.6	378.69	-9.1 ± 3.1	-143.92
4	1556-1829	10	395.0 ± 5.6	378.69	-9.1 ± 3.1	-143.92

\* Points rejected due to failure of statistical test

The data of Yanes *et al.* [1] are in good agreement with the adopted  $\Delta H^\circ(298.15\text{ K})$  values due to standard calorimetric measurements.

West Cannanby and Entrance

**Heat Capacity and Entropy** The low temperature heat capacity of  $\alpha$ -Be<sub>2</sub>N<sub>2</sub> has been measured, 25–310 K, by Justice.<sup>5</sup> These measurements are joined smoothly with the high temperature enthalpies reported by Douglas and Payne.<sup>6</sup> Above 1200 K the values were smoothly extrapolated to a limiting value of  $6.2 \text{ cal K}^{-1} \text{ g-atom}^{-1}$ . The entropy at 298.15 K was calculated by integration of the low temperature data based on  $S(25 \text{ K}) = 0.002$

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Fusion Data

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## References

References  
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<sup>1A</sup> J. L. Vial, *J. Am. Chem. Soc.*, **100**, 30-32 (1978).

<sup>1B</sup> F. E. Hayes, M. A. Greenbaum, and M. Enser, *J. Phys. Chem.*, **68**, 2682 (1964).

K. E. Tales, M. A. Utechtzamli and M. Farber, J. Phys. Chem. 68, 2882 (1964).

SB Justice The Dow Chemical Company, Oneonta, Pennsylvania under contract AFOSR-67-C-0000 (Amendment 1967)

B. H. Justice, The Dow Chemical Co., Ist. Quarterly Report Under Contract AF04-75B-111 S No. Buu. Signed Report 7587 (July 1962)

J. B. Douglas and W. R. Payne, U. S. Natl. Bur. Stand. Report 1287, July 1902.

Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $P^* = 0.1\text{ MPa}$			
$T/\text{K}$	$C_p^*$ $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$S^*$ $[\text{J}^*\cdot\text{K}^{-1}\cdot\text{mol}^{-1}]$	$H^* - H^*(T_r)$ $\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_H^*$ $\text{kJ}\cdot\text{mol}^{-1}$	$\Delta_G^*$ $\text{kJ}\cdot\text{mol}^{-1}$
0	0	0	-7.075	-580.879	-580.879
100	6.109	13.845	-6.933	-583.756	-567.089
200	35.489	14.313	-6.962	-586.429	-550.790
298.15	64.358	34.129	0.	-588.270	-532.874
300	64.668	34.528	0.119	-588.296	-532.530
400	84.433	56.036	36.928	-589.216	-513.778
500	97.512	76.374	42.811	-589.325	-67.092
600	106.516	94.995	49.281	27.009	-494.891
700	112.922	111.922	57.640	37.988	-588.882
800	117.591	127.321	65.402	49.535	-587.172
900	121.043	141.381	71.075	61.475	-586.186
1000	123.612	154.273	80.559	73.714	-585.237
1100	125.520	166.148	87.807	86.174	-584.387
1200	126.922	177.132	94.799	98.800	-583.685
1300	127.976	187.333	101.530	111.515	-583.169
1400	128.616	196.840	108.002	124.374	-582.871
1500	129.047	205.730	114.224	137.259	-582.816
1600	129.269	214.066	120.206	150.176	-626.634
1700	129.319	221.905	125.060	163.106	-625.974
1800	129.366	229.298	131.498	176.040	-625.298
1900	129.411	236.293	136.631	188.579	-624.733
2000	129.452	242.932	141.971	201.922	-624.286
2100	129.490	249.249	146.931	214.869	-623.896
2200	129.536	255.274	151.720	227.820	-623.582
2300	129.559	261.032	156.148	240.774	-623.343
2400	129.588	266.547	160.826	253.731	-623.176
2473.000	129.606	270.430	164.004	263.192	-623.000
2500	129.615	271.838	165.161	266.692	-623.083
2600	129.639	276.922	169.362	279.654	-623.062
2700	129.659	281.815	173.437	292.619	-623.112
2800	129.677	286.530	177.293	305.586	-1492.105
2900	129.692	291.081	181.235	318.555	-1493.106
3000	129.704	295.478	184.970	331.524	-1490.129

**Beryllium Nitride ( $\text{Be}_3\text{N}_2$ )****Liquid****Beryllium Nitride ( $\text{Be}_3\text{N}_2$ )**

$S^\circ(298.15 \text{ K}) = [39.457] \text{ J K}^{-1} \cdot \text{mol}^{-1}$   
 $T_{\text{fus}} = 2473 \text{ K}$

**Enthalpy of Formation**

The enthalpy of formation of  $\text{Be}_3\text{N}_2(\text{O})$  is calculated from that of the crystal by adding  $\Delta_{\text{fus}}H^\circ$  and the difference in enthalpy,  $H^\circ(298.15 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and liquid.

**Heat Capacity and Entropy**

The heat capacity is estimated to be constant and slightly greater than the maximum for  $\text{Be}_3\text{N}_2(\text{cr})$ . The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

**Fusion Data**

The melting point was reported by Fichter and Brunner.<sup>1</sup> The enthalpy of melting is calculated on the assumption that each g-atom contributed 2.5 cal K<sup>-1</sup> mol<sup>-1</sup> to  $\Delta_{\text{fus}}S^\circ$ .

**References**

[F. Fichter and E. Brunner, Z. anorg. allgem. Chem. 93, 84 (1915).]

		$M_r = 55.04994$ Beryllium Nitride ( $\text{Be}_3\text{N}_2$ )			
		Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$			
		$\Delta H^\circ(298.15 \text{ K}) = [-486.979] \text{ kJ mol}^{-1}$	$\Delta_{\text{fus}}H^\circ = [129.3] \text{ kJ mol}^{-1}$	$S^\circ = -[G^\circ - H^\circ(T_r)]/T_r$	$H^\circ - H^\circ(T_r)/T_r$
$T/K$	$C_p^*$	$\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$	$\text{J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$	$\text{J} \cdot \text{mol}^{-1}$	$\text{kJ} \cdot \text{mol}^{-1}$
100	0				
200	298.15	133.888	39.457	39.457	0.
300	133.888	40.285	39.459	0.248	-486.979
400	133.888	78.802	44.711	13.636	-432.838
500	133.888	108.678	54.628	27.025	-415.600
600	133.888	133.089	65.732	40.414	-477.790
700	133.888	153.728	76.867	53.803	-463.172
800	133.888	171.606	87.617	67.192	75.890
900	133.888	187.376	97.842	80.580	75.364
1000	133.888	201.482	107.513	93.969	42.272
1100	133.888	214.243	116.645	107.913	41.736
1200	133.888	228.893	125.271	120.747	33.447
1300	133.888	246.610	133.429	134.126	27.569
1400	133.888	246.532	141.157	147.524	23.189
1500	133.888	253.769	148.494	160.913	19.800
1600	133.888	264.410	155.471	174.302	17.103
1700	133.888	272.527	162.121	187.561	14.905
1800	133.888	281.180	168.469	201.080	13.889
1900	133.888	287.419	174.541	214.468	13.080
2000	133.888	292.287	180.358	212.837	11.541
2100	133.888	300.819	185.940	241.246	10.224
2200	133.888	307.047	191.304	234.635	9.084
2300	133.888	312.999	196.467	268.024	8.036
2400	133.888	318.1697	201.442	281.412	7.075
2473.000	133.888	322.709	204.963	291.186	6.222
-- CRYSTAL <-> LIQUID ---					
2500	133.888	324.163	206.242	294.801	4.777
2600	133.888	329.414	210.879	308.190	-493.682
2700	133.888	334.667	215.384	321.579	-493.235
2800	133.888	339.336	219.705	334.968	-492.861
2900	133.888	344.034	223.911	348.376	-395.432
3000	133.888	348.573	227.992	361.745	-362.013
3100	133.888	352.964	231.953	375.134	-135.246
3200	133.888	357.214	235.801	388.523	-131.905
3300	133.888	361.334	239.543	348.597	-137.731
3400	133.888	363.331	243.184	401.912	-142.6
3500	133.888	365.212	246.730	415.360	-3.726
3600	133.888	367.084	250.185	428.689	-134.210
3700	133.888	372.984	253.553	442.078	289.194
3800	133.888	380.223	256.840	468.836	335.758
3900	133.888	383.701	260.048	482.244	-132.973
4000	133.888	387.091	263.182	495.653	-132.682

PREVIOUS: September 1964

CURRENT: March 1967

CRYSTAL( $\alpha$ )-LIQUIDBeryllium Nitride ( $\text{Be}_3\text{N}_2$ ) $M_r = 55.04994$  Beryllium Nitride ( $\text{Be}_3\text{N}_2$ )

0 to 2473 K  
above 2473 K  
crystal, alpha  
liquid

Refer to the individual tables for details.

$T/K$	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$			Standard State Pressure = $P^\circ = 0.1 \text{ MPa}$		
		$J/\text{K}^{-1}\text{mol}^{-1}$	$S^\circ - [C^\circ - H^\circ(T)/T]/T$	$H^\circ - H^\circ(T)/T$	$\Delta H^\circ$	$\Delta G^\circ$	$\log K_t$
0	0	0	0	-7.075	-580.879	-580.879	INFINITE
100	6.109	1.845	71.174	-6.933	-583.756	-567.809	266.593
200	35.489	14.313	39.125	-4.962	-586.429	-550.790	143.852
298.15	64.358	34.129	0	-0.270	-588.270	-532.874	93.357
300	64.668	34.528	34.130	0.119	-588.296	-532.530	92.722
400	84.433	56.036	36.928	7.643	-589.216	-513.778	67.092
500	97.512	76.374	42.811	16.782	-589.325	-494.891	51.701
600	106.516	94.995	49.981	27.009	-588.882	-476.039	41.443
700	112.922	111.922	57.640	37.986	-588.110	-457.290	34.123
800	117.591	127.321	65.402	49.535	-587.172	-438.664	28.642
900	121.043	141.381	73.075	61.475	-586.186	-420.159	24.385
1000	123.612	154.273	80.539	73.714	-585.237	-401.763	20.986
1100	125.520	166.148	87.807	86.174	-584.387	-383.458	18.209
1200	126.622	177.132	94.799	98.800	-583.685	-365.224	15.898
1300	127.926	187.333	101.530	111.545	-583.169	-347.041	13.944
1400	128.616	196.840	108.002	124.374	-582.871	-328.890	12.271
1500	129.047	205.730	114.224	137.259	-582.816	-310.752	10.821
1600	129.269	214.086	120.206	150.176	-582.634	-291.033	9.501
1700	129.319	221.905	125.960	163.106	-582.924	-270.080	8.299
1800	129.366	229.298	131.498	176.040	-582.298	-249.166	7.231
1900	129.411	236.293	136.831	188.979	-624.753	-228.385	6.276
2000	129.452	242.932	141.971	201.922	-624.236	-207.431	5.418
2100	129.490	249.249	146.931	214.859	-623.896	-186.598	4.641
2200	129.525	255.274	151.720	227.820	-623.582	-165.782	3.926
2300	129.558	261.032	156.348	240.774	-623.343	-144.978	3.293
2400	129.587	266.547	160.826	253.731	-623.177	-124.184	2.703
2473.000	129.606	270.430	164.004	263.192	CRYSTAL <-> LIQUID		
2473.000	133.888	322.709	164.004	392.477	CRYSTAL <-> LIQUID		
2500	133.888	324.163	165.726	396.092	-493.682	-104.807	2.190
2600	133.888	329.414	171.921	409.481	-493.235	-89.261	1.793
2700	133.888	334.467	177.848	412.870	-492.861	-75.731	1.426
2800	133.888	339.336	183.529	436.259	-1365.432	-39.545	0.738
2900	133.888	344.034	188.984	449.647	-1362.013	-7.747	-0.140
3000	133.888	348.573	194.228	463.036	-1338.617	54.923	-0.956
3100	133.888	352.964	199.278	476.425	-1355.246	101.985	-1.718
3200	133.888	357.214	204.148	489.814	-1351.905	148.939	-2.431
3300	133.888	361.334	208.849	503.203	-1348.597	193.789	-3.099
3400	133.888	365.331	213.393	516.591	-1345.327	242.539	-3.726
3500	133.888	369.212	217.789	529.980	-1342.101	289.194	-4.316
3600	133.888	372.984	222.048	543.369	-1338.923	335.758	-4.872
3700	133.888	376.653	226.177	556.738	-1335.801	382.233	-5.396
3800	133.888	380.223	230.184	570.147	-1332.738	428.626	-5.892
3900	133.888	383.701	234.076	583.535	-1329.743	474.938	-6.361
4000	133.888	387.691	237.860	596.974	-1326.820	521.175	-6.806

PREVIOUS: CURRENT: March 1967  
 $\text{Be}_3\text{N}_2(\text{cr},)$

## IDEAL GAS

 $\text{M}_r = 75.03474$  Beryllium Oxide ((BeO)<sub>3</sub>)Beryllium Oxide ((BeO)<sub>3</sub>) $\text{Be}_3\text{O}_3(\text{g})$ 

$$\Delta_f H^\circ(0 \text{ K}) = -1049 \pm 38 \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = -1054 \pm 38 \text{ kJ} \cdot \text{mol}^{-1}$$

## Vibrational Frequencies and Degeneracies

v, cm <sup>-1</sup>	u, cm <sup>-1</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K				Standard State Pressure = p <sup>*</sup> = 0.1 MPa			
		C <sub>p</sub> <sup>r</sup>	J·K <sup>-1</sup> ·mol <sup>-1</sup>	S <sup>r</sup>	-(G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ))/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	ΔH <sup>r</sup>	ΔG <sup>r</sup>	log K <sub>r</sub>
0	0	0	0	0	INFINITE	-13.325	-1048.871	-1048.871	INFINITE
100	37,082	221,244	20,244	320,437	-7.919	-1049.940	-1045.917	-1045.917	546,331
200	50,124	250,834	278,210	-5,575	-1051,695	-1041,313	-217,963	-217,963	278,750
250	56,935	262,750	274,345	-2,899	-1052,582	-1038,572	-216,998	-216,998	278,750
298.15	63,458	272,337	273,337	0.	-1054,368	-1035,673	181,446	-1035,557	180,306
300	63,706	273,331	273,339	0.18	-1054,423	-1035,557	180,406	-1035,557	180,306
350	70,315	284,051	274,139	3.499	-1053,921	-1032,294	154,061	-1032,294	154,061
400	76,597	292,854	275,995	7.144	-1057,380	-1028,818	134,950	-1028,818	134,950
450	82,418	303,217	278,504	11,121	-1058,758	-1025,165	118,998	-1025,165	118,998
500	87,701	312,179	281,426	15,376	-1060,043	-1021,362	106,701	-1021,362	106,701
600	96,611	328,989	287,973	24,610	-1062,350	-1013,404	88,225	-1013,404	88,225
700	103,530	344,425	294,950	34,632	-1064,384	-1005,082	75,000	-1005,082	75,000
800	108,857	358,612	302,034	46,263	-1066,249	-996,482	65,064	-996,482	65,064
900	112,975	371,682	309,056	56,363	-1068,815	-987,653	57,322	-987,653	57,322
1000	116,187	383,758	315,930	67,838	-1069,812	-978,627	51,118	-978,627	51,118
1100	118,723	394,955	322,612	79,578	-1071,639	-969,420	46,034	-969,420	46,034
1200	120,750	403,376	329,079	91,556	-1073,559	-960,044	41,790	-960,044	41,790
1300	123,389	413,227	335,760	103,715	-1075,609	-950,502	38,192	-950,502	38,192
1400	127,730	424,229	341,355	116,024	-1077,818	-940,797	35,102	-940,797	35,102
1500	124,840	432,804	347,168	128,454	-1080,212	-930,927	32,418	-930,927	32,418
1600	125,766	440,892	352,776	140,985	-1082,417	-919,315	30,013	-919,315	30,013
1700	126,547	448,540	358,186	153,602	-1082,033	-906,321	27,848	-906,321	27,848
1800	127,210	453,495	363,409	166,291	-1082,677	-893,233	25,921	-893,233	25,921
1900	127,778	462,686	368,454	179,041	-1131,159	-880,031	24,194	-880,031	24,194
2000	128,268	469,253	373,331	191,844	-1133,088	-866,780	22,638	-866,780	22,638
2100	128,694	475,522	378,049	204,692	-1134,870	-853,421	21,228	-853,421	21,228
2200	129,065	481,517	382,617	217,581	-1136,711	-859,974	19,944	-859,974	19,944
2300	129,391	487,262	387,043	230,504	-1138,615	-856,445	18,769	-856,445	18,769
2400	129,679	492,775	391,334	243,458	-1140,387	-812,830	17,691	-812,830	17,691
2500	129,933	498,074	395,499	256,439	-1142,629	-799,132	16,697	-799,132	16,697
2600	130,162	503,175	399,542	269,444	-1144,143	-771,351	15,778	-771,351	15,778
2700	130,366	508,091	403,472	282,470	-1146,932	-771,492	14,925	-771,492	14,925
2800	130,549	512,835	407,294	295,516	-1152,067	-738,872	13,784	-738,872	13,784
2900	130,713	517,419	411,613	308,579	-202,218	-693,039	11,270	-693,039	11,270
3000	130,862	521,833	414,634	321,658	-202,998	-647,274	11,270	-647,274	11,270
3100	130,997	526,147	418,162	343,751	-2019,610	-601,516	10,135	-601,516	10,135
3200	131,120	530,307	421,602	347,557	-2018,560	-553,784	9,072	-553,784	9,072
3300	131,232	534,344	424,958	360,975	-2018,151	-510,075	8,074	-510,075	8,074
3400	131,353	538,263	428,233	374,104	-2016,489	-464,384	7,134	-464,384	7,134
3500	131,429	542,072	431,431	387,242	-2016,379	-418,715	6,249	-418,715	6,249
3600	131,516	545,775	434,556	400,389	-2016,327	-373,060	5,413	-373,060	5,413
3700	131,595	549,380	437,611	413,545	-2015,339	-327,422	4,622	-327,422	4,622
3800	131,669	552,890	440,599	426,708	-2015,420	-281,793	3,874	-281,793	3,874
3900	131,737	556,311	443,522	439,878	-2015,078	-236,176	3,163	-236,176	3,163
4000	131,800	559,647	446,384	453,055	-2014,817	-190,567	2,489	-190,567	2,489
4100	131,859	562,903	449,186	468,238	-2014,646	-144,963	1,847	-144,963	1,847
4200	131,914	566,081	451,932	479,427	-2014,569	-99,362	1,236	-99,362	1,236
4300	131,964	569,185	454,622	492,621	-2014,594	-53,761	0,653	-53,761	0,653
4400	132,012	572,220	457,261	505,520	-2014,728	-8,160	-2,455	-8,160	-2,455
4500	132,036	575,187	460,544	519,023	-2014,975	37,446	-0,435	37,446	-0,435
4600	132,098	578,090	462,388	532,231	-2015,542	83,038	-0,943	83,038	-0,943
4700	132,137	580,931	464,880	545,443	-2015,836	128,682	-1,430	128,682	-1,430
4800	132,173	583,714	467,332	558,638	-2016,461	174,316	-1,897	174,316	-1,897
4900	132,208	586,439	469,730	571,877	-2017,224	219,966	-2,345	219,966	-2,345
5000	132,240	589,111	472,091	585,100	-2018,130	265,632	-2,775	265,632	-2,775
5100	132,271	591,730	474,411	598,325	-2019,182	311,318	-3,189	311,318	-3,189
5200	132,299	594,298	476,632	601,554	-2020,387	357,023	-3,586	357,023	-3,586
5400	132,352	599,292	481,141	615,255	-2024,949	448,516	-4,339	448,516	-4,339
5500	132,376	601,721	483,311	651,255	-2024,949	494,304	-4,693	494,304	-4,693
5600	132,399	604,106	485,447	664,494	-2026,798	540,126	-5,038	540,126	-5,038
5700	132,421	606,450	487,549	677,735	-2028,815	585,981	-5,370	585,981	-5,370
5800	132,442	608,753	489,619	690,978	-2031,003	631,875	-5,691	631,875	-5,691
5900	132,462	611,017	491,658	704,224	-2033,164	677,904	-6,001	677,904	-6,001
6000	132,480	613,244	493,665	717,471	-2033,500	723,779	-6,301	723,779	-6,301

PREVIOUS September 1963 (1 atm)

CURRENT September 1963 (1 bar)

## NIST-JANAF THERMOCHEMICAL TABLES

 $\text{Be}_4\text{O}_4(\text{g})$  $M_f = 100.04632$  Beryllium Oxide ((BeO)<sub>4</sub>)

## IDEAL GAS

$$\Delta_f H^\circ(298.15 \text{ K}) = [302.6] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = -1581 \pm 50 \text{ kJ}\cdot\text{mol}^{-1}$$

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

$v$ , cm <sup>-1</sup>	$\nu$ , cm <sup>-1</sup>	$C''$	$J\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$S^\circ$	$-(C^\circ - H^\circ(T_r))/T$	$H^\circ - H^\circ(T_r)/T$	$\Delta_H^\circ$	$\Delta G^\circ$	$\log K_r$
0	0	0.000	0.000	INFINITE	-1581.354	-1581.354	-1581.354	-1581.354	INFINITE
100	43.449	2345.990	364.943	-12.895	-1583.686	-1572.422	-1572.422	-1560.180	821.349
200	64.574	272.167	305.947	-7.536	-1586.479	-1586.479	-1586.479	-1586.479	407.477
250	77.225	287.926	303.979	-4.013	-1588.220	-1586.405	-1586.405	-1586.405	324.566
298.15	89.389	302.575	302.575	0.000	-1589.920	-1546.545	-1546.545	-1546.545	270.948
300	89.844	303.129	302.577	.166	-1589.985	-1546.276	-1546.276	-1546.276	269.231
350	101.591	317.876	303.714	10.303	-1593.157	-1531.209	-1531.209	-1531.209	199.955
400	112.062	332.240	306.381	16.140	-1594.463	-1523.385	-1523.385	-1523.385	176.830
450	121.155	345.377	310.012	22.397	-1595.572	-1515.425	-1515.425	-1515.425	158.315
500	129.942	359.056	314.262	29.237	-1597.439	-1499.211	-1499.211	-1499.211	130.518
600	141.187	383.708	323.813	35.937	-1598.930	-1482.718	-1482.718	-1482.718	110.642
700	150.034	406.173	333.999	50.522	-1600.247	-1466.076	-1466.076	-1466.076	95.722
800	156.507	426.652	344.320	65.865	-1601.525	-1449.171	-1449.171	-1449.171	84.108
900	161.327	445.377	354.524	81.768	-1602.838	-1432.173	-1432.173	-1432.173	74.809
1000	164.987	462.573	364.881	98.092	-1604.314	-1415.034	-1415.034	-1415.034	67.194
1100	167.817	478.436	374.129	114.738	-1604.314	-1415.034	-1415.034	-1415.034	60.843
1200	170.043	493.137	383.441	131.635	-1605.947	-1397.757	-1397.757	-1397.757	55.463
1300	171.821	506.521	392.412	148.732	-1607.797	-1380.334	-1380.334	-1380.334	50.845
1400	173.262	519.628	401.045	165.988	-1609.887	-1362.760	-1362.760	-1362.760	45.838
1500	174.443	531.604	405.354	183.275	-1612.275	-1345.026	-1345.026	-1345.026	43.258
1600	175.422	542.894	417.350	200.870	-1673.096	-1325.021	-1325.021	-1325.021	40.043
1700	176.245	551.555	425.052	218.455	-1674.488	-1307.224	-1307.224	-1307.224	37.184
1800	176.940	563.549	432.474	216.115	-1675.938	-1281.344	-1281.344	-1281.344	34.623
1900	177.533	573.232	439.632	253.839	-1677.457	-1259.381	-1259.381	-1259.381	32.316
2000	178.043	582.551	446.342	271.619	-1679.033	-1237.356	-1237.356	-1237.356	
2100	178.484	591.049	453.218	289.446	-1680.734	-1215.209	-1215.209	-1215.209	30.227
2200	178.869	598.361	459.673	307.314	-1682.505	-1192.999	-1192.999	-1192.999	28.375
2300	179.205	607.220	465.921	325.218	-1684.371	-1170.708	-1170.708	-1170.708	26.588
2400	179.502	614.953	471.972	343.154	-1686.335	-1148.334	-1148.334	-1148.334	24.993
2500	179.765	622.286	477.839	361.377	-1688.402	-1125.375	-1125.375	-1125.375	23.524
2600	179.998	629.141	483.531	379.106	-1690.573	-1103.332	-1103.332	-1103.332	22.166
2700	180.207	636.38	489.058	397.116	-1692.849	-1080.702	-1080.702	-1080.702	20.907
2800	180.394	642.696	494.429	415.146	-1694.061	-1033.096	-1033.096	-1033.096	19.273
2900	180.563	649.029	499.652	431.194	-1697.299	-967.916	-967.916	-967.916	17.454
3000	180.715	655.153	504.733	451.258	-1695.580	-902.933	-902.933	-902.933	15.719
3100	180.853	661.081	509.682	469.337	-1693.908	-833.727	-833.727	-833.727	14.116
3200	180.979	666.325	514.503	487.429	-1692.290	-782.015	-782.015	-782.015	12.613
3300	181.093	672.395	519.204	505.522	-1690.711	-707.755	-707.755	-707.755	4.270
3400	181.198	677.803	522.189	523.647	-1692.837	-642.837	-642.837	-642.837	9.876
3500	181.294	683.057	528.265	541.772	-1694.219	-284.819	-284.819	-284.819	6.626
3600	181.382	688.166	532.636	559.905	-1696.479	-284.003	-284.003	-284.003	1.552
3700	181.463	693.346	536.907	567.047	-1697.047	-60.107	-60.107	-60.107	-6.094
3800	181.538	697.977	541.083	596.198	-1698.336	-448.334	-448.334	-448.334	6.329
3900	181.607	702.693	545.166	614.355	-1699.620	-382.567	-382.567	-382.567	5.272
4000	181.671	707.292	549.162	632.519	-1700.714	-284.015	-284.015	-284.015	4.270
4100	181.731	711.779	553.074	650.689	-1701.252	-189.432	-189.432	-189.432	2.413
4200	181.787	716.158	558.905	668.865	-1702.559	-124.763	-124.763	-124.763	1.552
4300	181.838	720.437	560.653	687.047	-1703.233	-283.959	-283.959	-283.959	-283.959
4500	181.931	728.706	567.936	696.198	-1703.424	-284.466	-284.466	-284.466	-284.466
5000	182.118	747.384	584.996	714.438	-1704.336	-392.368	-392.368	-392.368	-392.368
5100	182.199	751.493	591.493	732.652	-1704.454	-457.036	-457.036	-457.036	-457.036
5200	182.178	755.028	591.400	735.868	-1704.462	-521.720	-521.720	-521.720	-521.720
5300	182.205	758.499	594.420	739.818	-1704.482	-586.630	-586.630	-586.630	-586.630
5400	182.231	761.903	597.588	743.309	-1704.517	-631.162	-631.162	-631.162	-631.162
5500	182.256	765.249	600.606	748.021	-1704.535	-626.071	-626.071	-626.071	-626.071
5600	182.279	768.533	603.576	753.760	-1704.556	-780.718	-780.718	-780.718	-780.718
5700	182.301	771.759	606.998	761.969	-1704.576	-843.547	-843.547	-843.547	-843.547
5800	182.322	774.930	609.375	769.020	-1704.595	-910.418	-910.418	-910.418	-910.418
5900	182.342	778.047	612.207	778.454	-1704.614	-975.326	-975.326	-975.326	-975.326
6000	182.361	781.112	614.997	796.659	-1704.633	-1040.285	-1040.285	-1040.285	-1040.285

CURRENT: September 1963 (1 atm)

PREVIOUS: September 1963 (1 atm)

 $\text{Be}_4\text{O}_4(\text{g})$  $\text{Be}_4\text{O}_4(\text{g})$ 

**Enthalpy of Formation**  
 Chupka, Berkowitz, and Giese<sup>1</sup> measured the variation of intensity of the (BeO)<sub>4</sub><sup>+</sup> ion with temperature in a mass spectrometer. They reported a 2nd law enthalpy of vaporization of 177 ± 8 kcal·mol<sup>-1</sup> at 2150 K, which included an approximate correction of 9 kcal·mol<sup>-1</sup>, and this value was adopted here.

**Heat Capacity and Entropy**

The assumed D<sub>4h</sub> structure has 14 vibrational frequencies of the type 2A<sub>1g</sub>, A<sub>2g</sub>, 2B<sub>1g</sub>, E<sub>g</sub>, A<sub>3g</sub>, B<sub>2g</sub>, B<sub>3g</sub>, and 3E<sub>u</sub>. The frequencies were estimated by comparison with (BeO)<sub>1</sub> and cyclobutane from Rathjens, Freeman, and Pitzer.<sup>2</sup> The estimated structure and frequencies gave an entropy which was in excellent agreement with the experimental enthalpy and equilibrium constant determined by Chupka et al.<sup>1</sup> The bond lengths were taken equal to those in Be<sub>2</sub>O<sub>4</sub>(g) and the angles<sup>3</sup> were chosen so that O-Be-O was almost linear. The principal moments of inertia are  $I_A = I_B = 38.2258 \times 10^{-39} \text{ g} \cdot \text{cm}^2$ , and  $I_C = 76.4515 \times 10^{-39} \text{ g} \cdot \text{cm}^2$ .

**References**

- <sup>1</sup>W. A. Chupka, J. Berkowitz, and C. F. Giese, J. Chem. Phys., 30, 827 (1959).
- <sup>2</sup>G. W. Rathjens, N. K. Freeman, W. D. Gwinn, and K. S. Pitzer, J. Am. Chem. Soc., 75, 5634 (1953).

**Heat Capacity and Entropy**

The assumed D<sub>4h</sub> structure has 14 vibrational frequencies of the type 2A<sub>1g</sub>, A<sub>2g</sub>, 2B<sub>1g</sub>, E<sub>g</sub>, A<sub>3g</sub>, B<sub>2g</sub>, B<sub>3g</sub>, and 3E<sub>u</sub>. The frequencies were estimated by comparison with (BeO)<sub>1</sub> and cyclobutane from Rathjens, Freeman, and Pitzer.<sup>2</sup> The estimated structure and frequencies gave an entropy which was in excellent agreement with the experimental enthalpy and equilibrium constant determined by Chupka et al.<sup>1</sup> The bond lengths were taken equal to those in Be<sub>2</sub>O<sub>4</sub>(g) and the angles<sup>3</sup> were chosen so that O-Be-O was almost linear. The principal moments of inertia are  $I_A = I_B = 38.2258 \times 10^{-39} \text{ g} \cdot \text{cm}^2$ , and  $I_C = 76.4515 \times 10^{-39} \text{ g} \cdot \text{cm}^2$ .

**References**

- <sup>1</sup>W. A. Chupka, J. Berkowitz, and C. F. Giese, J. Chem. Phys., 30, 827 (1959).
- <sup>2</sup>G. W. Rathjens, N. K. Freeman, W. D. Gwinn, and K. S. Pitzer, J. Am. Chem. Soc., 75, 5634 (1953).

Beryllium Oxide ((BeO)<sub>5</sub>)

## IDEAL GAS

## Enthalpy of Formation

$$\Delta H^\circ(298.15\text{ K}) = [323.28] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(0\text{ K}) = -2101 \pm 75 \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^\circ(298.15\text{ K}) = -2113 \pm 75 \text{ kJ}\cdot\text{mol}^{-1}$$

Vibrational Frequencies and Degeneracies	
v, cm <sup>-1</sup>	v, cm <sup>-1</sup>
[700] (1)	[1200] (2)
[850] (1)	[600] (2)
[1400] (1)	[500] (2)
[1100] (2)	[900] (1)
[1200] (2)	[200] (2)
[1000] (2)	[400] (2)
[1200] (2)	[500] (2)

Ground State Quantum Weight: [1]

Point Group: [D<sub>3h</sub>]

Bond Distance: Be—O = [1.63] Å

Bond Angles: Be—O—Be = [110°];

O—Be—O = [178°]; O—Be—O = [6.9690 X 10<sup>-12</sup>] g<sup>3</sup> cm<sup>6</sup>

## Enthalpy of Formation

Chupka, Berkowitz, and Giese<sup>1</sup> measured the variation in intensity of the (BeO)<sub>5</sub> ion with temperature in a mass spectrometer. They calculated a second law enthalpy of vaporization of 193 ± 12 kcal·mol<sup>-1</sup> at 2150 K, the uncertainty reflects the inclusion of an approximate correction of 10 kcal·mol<sup>-1</sup>. This value was adopted here.

## Heat Capacity and Entropy

The assumed D<sub>3h</sub> structure has 14 vibrations of the type 2A<sub>1</sub>, A<sub>1</sub>, 3E<sub>1</sub>, 4E<sub>2</sub>, A<sub>1'</sub>, E<sub>1'</sub>, and 2E<sub>2'</sub>. These were estimated by comparison with similar motions in other ring structures including (BeO)<sub>4</sub> and (BeO)<sub>6</sub>. The estimated structure and frequencies gave an entropy in good agreement with the experimental enthalpy and equilibrium constant determined by Chupka *et al.*<sup>1</sup>

The bond length was assumed to be the same as in Be<sub>2</sub>O<sub>3</sub>(g) and the angles were chosen so as to make O—Be—O almost linear. The principal moments of inertia are: I<sub>A</sub> = I<sub>B</sub> = 70.3689 × 10<sup>-39</sup>, and I<sub>C</sub> = 140.7378 × 10<sup>-39</sup> g·cm<sup>2</sup>.

## References

- <sup>1</sup>W. A. Chupka, J. Berkowitz, and C. F. Giese, *J. Chem. Phys.*, **30**, 827 (1959).

Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K			
T/K	C <sub>p</sub> /JK <sup>-1</sup> mol <sup>-1</sup>	S <sup>o</sup> /JK <sup>-1</sup> mol <sup>-1</sup>	H <sup>o</sup> —H <sup>o</sup> (T <sub>r</sub> )/kJ·mol <sup>-1</sup>
0	0	0	0
100	45.283	244.859	-19.090
200	77.909	285.714	-15.427
250	95.670	305.013	-9.345
289.15	112.018	323.278	-5.005
300	112.622	323.973	-2.111
350	128.074	342.516	0.208
400	141.704	360.528	6.232
450	153.478	377.916	12.985
500	163.529	394.621	20.372
600	179.296	425.099	33.014
700	190.665	454.448	45.488
800	198.713	480.478	56.017
900	205.156	504.288	67.520
1000	209.847	526.157	78.021
1100	213.474	546.335	87.741
1200	216.326	565.937	96.155
1300	218.603	582.445	104.572
1400	220.447	598.715	112.989
1500	221.960	613.978	121.396
1600	223.215	628.344	129.793
1700	224.267	641.909	138.196
1800	225.157	654.754	146.590
1900	225.916	666.948	154.982
2000	226.568	678.553	163.385
2100	227.132	689.621	171.729
2200	227.621	697.621	179.952
2300	228.053	706.199	188.263
2400	228.435	710.037	196.572
2500	228.771	729.373	204.881
2600	229.070	738.352	213.190
2700	229.337	747.002	221.499
2800	229.577	755.347	229.798
2900	229.792	763.407	238.097
3000	229.987	771.201	246.396
3100	230.164	784.745	254.695
3200	230.244	786.055	262.994
3300	230.471	793.145	271.293
3400	230.605	800.027	280.592
3500	230.727	806.313	288.891
3600	230.840	813.215	297.190
3700	230.944	819.341	305.489
3800	231.040	825.701	313.788
3900	231.128	831.304	322.087
4000	231.210	837.556	330.386
4100	231.287	843.266	338.685
4200	231.357	848.341	346.984
4300	231.424	854.285	355.283
4400	231.485	859.505	363.582
4500	231.543	864.869	371.881
4600	231.597	869.899	380.180
4700	231.647	874.880	388.479
4800	231.695	879.258	396.778
4900	231.739	884.526	405.077
5000	231.781	889.218	413.376
5100	231.821	893.808	421.675
5200	231.858	898.310	429.974
5300	231.893	902.727	438.273
5400	231.926	907.062	446.572
5500	231.958	911.317	454.871
5600	231.988	915.997	463.170
5700	232.016	919.604	471.469
5800	232.043	923.639	479.768
5900	232.068	927.606	488.067
6000	232.093	931.506	496.366

CURRENT: September 1963 (1 bar)

PREVIOUS: September 1963 (1 atm)

Beryllium Oxide ((BeO)<sub>5</sub>)Be<sub>5</sub>O<sub>5</sub>(g)

Beryllium Oxide ((BeO)<sub>6</sub>)

## IDEAL GAS

*M<sub>r</sub>* = 150.06948 Beryllium Oxide ((BeO)<sub>6</sub>)

$$S^{\circ}(298.15\text{ K}) = [343.2] \text{ J K}^{-1} \text{ mol}^{-1}$$

$$\Delta H^{\circ}(0\text{ K}) = -2645 \pm 92 \text{ kJ mol}^{-1}$$

$$\Delta H^{\circ}(298.15\text{ K}) = -2661 \pm 92 \text{ kJ mol}^{-1}$$

Vibrational Frequencies and Degeneracies	$\sigma = [12]$
$v, \text{ cm}^{-1}$	$v, \text{ cm}^{-1}$
$u, \text{ cm}^{-1}$	$u, \text{ cm}^{-1}$
$[700] (1) [600] (2)$	$[900] (1) [1100] (2)$
$[850] (1) [750] (2)$	$[1100] (1) [1200] (2)$
$[400] (1) [850] (2)$	$[1000] (1) [500] (2)$
$[500] (1) [850] (2)$	$[200] (1) [200] (2)$
$[400] (1) [950] (2)$	$[1400] (1) [250] (2)$

Point Group: D<sub>6h</sub>  
 Bond Distance: Be–O = [1.63] Å  
 Bond Angles: Be–O–Be = [110]<sup>o</sup>, O–Be–O = [190]<sup>o</sup>  
 Product of the Moments of Inertia:  $I_A I_B I_C = [3.1282 \times 10^{-11}] \text{ g cm}^6$

$\sigma = [12]$

## Enthalpy of Formation

Chupka, Berkowitz, and Giese<sup>1</sup> measured the temperature dependence of the (BeO)<sub>6</sub> ion in a mass spectrometer. They calculated a 2nd law enthalpy of vaporization of  $203 \pm 15 \text{ kcal mol}^{-1}$  which was adopted here. The uncertainty reflects in part an approximate correction of 10 kcal·mol<sup>-1</sup> and the small observed intensities.

## Heat Capacity and Entropy

The assumed symmetry D<sub>6h</sub> has 20 vibrational frequencies of the type 2A<sub>1g</sub>, A<sub>2g</sub>, B<sub>1g</sub>, B<sub>2g</sub>, E<sub>1g</sub>, 4E<sub>2g</sub>, A<sub>2u</sub>, 2B<sub>1u</sub>, 2B<sub>2u</sub>, 3E<sub>1u</sub>, and 2E<sub>2u</sub>. The frequencies were estimated by comparison with similar motions in other ring molecules including benzene, (BeO)<sub>4</sub>, and (BeO)<sub>4</sub>. The assumed structure and vibrational frequencies gave an entropy in good agreement with the experimental enthalpy and equilibrium constant determined by Chupka *et al.*<sup>1</sup> The bond length was taken equal to that in Be<sub>2</sub>O<sub>2</sub>(g). The angles were chosen so that the O–Be–O angle was almost linear but with the Be–O–Be angle less than 120°. The principal moments of inertia are:  $I_A = I_B = 116.0793 \times 10^{-39}$ , and  $I_C = 232.1586 \times 10^{-39}$  g·cm<sup>2</sup>.

## References

W. A. Chupka, J. Berkowitz, and C. F. Giese, *J. Chem. Phys.*, **30**, 827 (1959).

T/K	$C_p^{\circ}$	$S^{\circ}$	$-[G^{\circ} - H^{\circ}(T)]/T$	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		$H^{\circ} - H^{\circ}(T_r)$	$\Delta H^{\circ}$	Standard State Pressure = $P^{\circ} = 0.1 \text{ MPa}$	$\log K_r$
				$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$				
0	0	0	INFINITE	-21.479	-2644.860	-2644.860	-2644.860	INFINITE	
100	50.386	253.784	430.456	-17.667	-2649.997	-2623.081	-1370.157		
200	88.526	299.761	353.847	-10.817	-2655.247	-2594.199	-577.535		
250	10.694	321.887	345.242	-5.839	-2658.293	-2578.570	-538.763		
298.15	131.624	343.191	343.191	0.	-2661.024	-2562.357	-449.021		
300	132.400	344.008	344.194	0.244	-2661.125	-2562.357	-446.146		
350	157.248	365.937	348.860	7.370	-2663.597	-2545.687	-379.923		
400	169.665	387.432	348.861	15.428	-2665.907	-2538.673	-330.211		
450	184.604	408.302	354.513	291.140	-2667.757	-2493.948	-291.516		
500	197.270	428.426	360.724	33.851	-2669.277	-2493.948	-260.341		
600	216.981	466.236	375.205	54.619	-2671.589	-2458.651	-214.045		
700	241.084	500.002	390.716	77.061	-2673.260	-2423.203	-180.808		
800	241.334	537.264	408.479	100.708	-2674.605	-2381.181	-155.867		
900	248.936	561.249	422.094	125.240	-2677.469	-2312.090	-136.459		
1000	254.690	587.789	437.353	150.434	-2677.134	-2315.178	-120.925		
1100	262.280	612.280	452.158	176.134	-2678.588	-2278.757	-108.209		
1200	262.617	634.983	466.459	202.228	-2680.289	-2242.336	-97.606		
1300	265.398	656.117	480.245	228.634	-2682.303	-2205.761	-88.629		
1400	267.849	675.878	493.520	255.290	-2684.682	-2169.017	-80.927		
1500	268.494	694.401	506.301	282.150	-2687.469	-2132.090	-74.246		
1600	271.024	711.844	518.608	309.179	-2777.915	-2091.808	-68.291		
1700	272.306	728.511	520.464	336.347	-2791.211	-2048.886	-62.955		
1800	273.389	743.911	541.892	363.633	-2793.633	-2048.590	-58.209		
1900	278.117	758.759	552.918	391.019	-2792.069	-1962.809	-53.961		
2000	275.107	772.809	563.563	418.491	-2783.660	-1919.649	-50.136		
2100	275.795	782.248	573.850	446.037	-2785.376	-1875.407	-46.673		
2200	276.393	799.092	583.798	473.647	-2787.224	-1833.078	-43.523		
2300	276.918	811.390	593.428	501.314	-2789.213	-1789.665	-40.645		
2400	277.379	821.786	602.757	529.029	-2791.348	-1746.162	-38.004		
2500	277.788	834.518	611.802	556.788	-2793.633	-1702.566	-35.773		
2600	278.152	845.420	620.579	584.585	-2796.076	-1658.875	-33.327		
2700	278.477	853.924	629.103	612.417	-2798.675	-1615.087	-31.246		
2800	278.768	866.056	631.385	640.279	-2801.776	-1533.865	-28.615		
2900	279.030	875.843	645.440	668.169	-2804.714	-1476.310	-25.691		
3000	279.267	883.307	653.279	696.084	-2808.316	-1430.316	-23.870		
3100	279.482	894.468	660.912	724.022	-2812.976	-1415.475	-20.414		
3200	279.677	903.344	668.350	731.980	-2817.742	-1404.324	-18.026		
3300	279.855	911.953	675.602	739.957	-2820.582	-1401.205	-15.784		
3400	280.018	920.310	682.677	807.951	-2827.521	-1377.177	-13.676		
3500	280.167	928.429	689.583	833.960	-2834.569	-1353.241	-11.689		
3600	280.304	936.324	696.328	863.984	-2851.736	-1316.385	-9.814		
3700	280.430	944.005	702.919	892.021	-2872.572	-1289.609	-8.041		
3800	280.547	951.486	709.362	920.069	-2891.475	-1262.954	-7.363		
3900	280.654	958.774	715.664	948.130	-2901.742	-1246.777	-6.772		
4000	280.754	965.881	721.831	971.200	-2911.833	-1230.582	-6.260		
4100	280.847	972.815	727.868	1004.280	-2920.280	-1217.747	-5.824		
4200	280.933	979.784	733.781	1032.369	-2930.911	-1207.847	-5.456		
4300	281.013	986.195	739.575	1060.467	-2940.252	-1197.770	-5.087		
4400	281.088	992.656	745.254	1088.572	-2950.811	-1187.171	-4.793		
4500	281.158	998.974	750.822	1116.684	-2963.599	-1172.541	-4.500		
4600	281.224	1003.154	756.284	1144.803	-2970.530	-1157.205	-4.216		
4700	281.285	1011.203	761.644	1177.929	-2977.200	-1141.833	-4.024		
4800	281.343	1017.126	766.905	1201.060	-2984.967	-1120.535	-3.824		
4900	281.397	1022.927	772.071	1229.197	-2991.294	-1107.847	-3.634		
5000	281.448	1028.613	777.145	1257.339	-3001.407	-1094.157	-3.438		
5100	281.496	1034.187	782.130	1285.487	-3010.817	-1080.473	-3.244		
5200	281.541	1039.633	787.030	1313.638	-3026.795	-1062.795	-3.050		
5300	281.584	1045.016	791.848	1341.795	-3030.556	-1053.141	-2.859		
5400	281.624	1050.280	796.955	1349.955	-3034.904	-1043.546	-2.654		
5500	281.663	1055.488	801.245	1348.120	-3045.577	-1045.893	-2.454		
5600	281.699	1060.524	805.829	1426.288	-3058.384	-1043.324	-2.254		
5700	281.733	1063.510	810.342	1454.459	-3072.920	-1041.920	-2.054		
5800	281.766	1070.410	814.783	1482.634	-3086.747	-1039.520	-1.854		
5900	281.797	1075.227	819.157	1510.812	-3101.517	-1037.127	-1.654		
6000	281.826	1079.963	823.464	1538.394	-3120.037	-1035.744	-1.454		

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

Be<sub>6</sub>O<sub>6</sub>(g)

Be<sub>6</sub>O<sub>6</sub>(g)

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- The entropy in the present table is higher by  $1.83 \text{ cal K}^{-1} \text{ mol}^{-1}$  at  $298.15 \text{ K}$  and  $1.76 \text{ cal K}^{-1} \text{ mol}^{-1}$  at  $1000 \text{ K}$  than that proposed by Jackson.<sup>9</sup> The moment of inertia as calculated by Jackson<sup>9</sup> appears to be in error.
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