Boron (B)

REFERENCE STATE

0	to	2350 K	crystal
2350	to 4137.895 K		liquid
above		137.895 K	ideal monatomic gas

Refer to the individual tables for details.

$_r$ = 10.81 Boron (B) B$_1$(ref)

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0	0.	0.	INFINITE	−1.214	0.	0.	0.
100	1.076	0.308	12.207	−1.190	0.	0.	0.
200	5.998	2.419	6.704	−0.857	0.	0.	0.
298.15	11.315	5.834	5.834	0.	0.	0.	0.
300	11.405	5.904	5.834	0.021	0.	0.	0.
400	15.693	9.794	6.335	1.384	0.	0.	0.
500	18.722	13.644	7.415	3.115	0.	0.	0.
600	20.778	17.251	8.758	5.096	0.	0.	0.
700	22.249	20.570	10.212	7.251	0.	0.	0.
800	23.361	23.617	11.699	9.534	0.	0.	0.
900	24.245	26.421	13.181	11.915	0.	0.	0.
1000	24.978	29.014	14.637	14.378	0.	0.	0.
1100	25.606	31.425	16.055	16.908	0.	0.	0.
1200	26.161	33.677	17.430	19.496	0.	0.	0.
1300	26.663	35.792	18.762	22.138	0.	0.	0.
1400	27.125	37.785	20.051	24.828	0.	0.	0.
1500	27.557	39.671	21.296	27.562	0.	0.	0.
1600	27.966	41.463	22.501	30.338	0.	0.	0.
1700	28.356	43.170	23.667	33.155	0.	0.	0.
1800	28.732	44.801	24.796	36.009	0.	0.	0.
1900	29.097	46.365	25.891	38.901	0.	0.	0.
2000	29.452	47.866	26.952	41.828	0.	0.	0.
2100	29.799	49.312	27.983	44.791	0.	0.	0.
2200	30.140	50.706	28.984	47.788	0.	0.	0.
2300	30.475	52.053	29.958	50.819	0.	0.	0.
2350.000	30.641	52.710	30.435	52.346		BETA <--> LIQUID	
2350.000	31.750	74.075	30.435	102.554		TRANSITION	
2400	31.750	74.744	31.351	104.142	0.	0.	0.
2500	31.750	76.040	33.113	107.317	0.	0.	0.
2600	31.750	77.285	34.788	110.492	0.	0.	0.
2700	31.750	78.483	36.384	113.667	0.	0.	0.
2800	31.750	79.638	37.909	116.842	0.	0.	0.
2900	31.750	80.752	39.367	120.017	0.	0.	0.
3000	31.750	81.828	40.764	123.192	0.	0.	0.
3100	31.750	82.869	42.106	126.367	0.	0.	0.
3200	31.750	83.877	43.396	129.542	0.	0.	0.
3300	31.750	84.854	44.637	132.717	0.	0.	0.
3400	31.750	85.802	45.834	135.892	0.	0.	0.
3500	31.750	86.723	46.989	139.067	0.	0.	0.
3600	31.750	87.617	48.105	142.242	0.	0.	0.
3700	31.750	88.487	49.185	145.417	0.	0.	0.
3800	31.750	89.334	50.231	148.592	0.	0.	0.
3900	31.750	90.158	51.244	151.767	0.	0.	0.
4000	31.750	90.962	52.227	154.942	0.	0.	0.
4100	31.750	91.746	53.181	158.117	0.	0.	0.
4139.449	31.750	92.050	53.550	159.369		LIQUID <--> IDEAL GAS	
4139.449	20.860	208.131	53.550	639.878		FUGACITY = 1 bar	
4200	20.870	208.434	55.781	641.141	0.	0.	0.
4300	20.887	208.925	59.337	643.229	0.	0.	0.
4400	20.906	209.405	62.742	645.319	0.	0.	0.
4500	20.928	209.875	66.006	647.410	0.	0.	0.
4600	20.952	210.336	69.139	649.504	0.	0.	0.
4700	20.979	210.786	72.148	651.601	0.	0.	0.
4800	21.009	211.228	75.041	653.700	0.	0.	0.
4900	21.042	211.662	77.825	655.803	0.	0.	0.
5000	21.078	212.087	80.506	657.909	0.	0.	0.
5100	21.117	212.505	83.090	660.018	0.	0.	0.
5200	21.160	212.916	85.583	662.132	0.	0.	0.
5300	21.206	213.319	87.989	664.251	0.	0.	0.
5400	21.255	213.716	90.313	666.374	0.	0.	0.
5500	21.308	214.107	92.561	668.502	0.	0.	0.
5600	21.365	214.491	94.735	670.635	0.	0.	0.
5700	21.425	214.870	96.839	672.775	0.	0.	0.
5800	21.489	215.243	98.877	674.921	0.	0.	0.
5900	21.557	215 611	100.853	677.073	0.	0.	0.
6000	21.628	215.974	102.768	679.232	0.	0.	0.

PREVIOUS: March 1979 (1 atm) CURRENT June 1983 (1 bar)

Boron, Beta–Rhombohedral (β–B) CRYSTAL(β) $A_r = 10.81$

$S°(298.15\ K) = 5.83 \pm 0.08\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 2350 \pm 50\ K$

$\Delta_f H°(0\ K) = 0\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ{\cdot}mol^{-1}$
$\Delta_{fus} H° = 50.2 \pm 1.7\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The adopted low temperature heat capacity values ($T < 298.15$ K) are based on the heat capacity studies of Biler,[1] [2] Johnston *et al.*,[3] and Bogdanov *et al.*[4] The adopted high temperature heat capacities ($T > 298.15$ K) are derived from the enthalpy studies of McDonald and Stull[5] and Stout *et al.*[6] The mathematical and graphical treatment of these five studies, providing experimental measurements in the 2–2218 K range, yield a continuous and smooth heat capacity curve. The resulting entropy, $S°(298.15\ K) = 5.83 \pm 0.08\ J{\cdot}K^{-1}{\cdot}mol^{-1}$, is $0.07\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ less than the CODATA recommended entropy[7] due to the differing interpretation of the C_p results for $T<50$ K. In this analysis, the scatter in the experimental data obscures any differences that may arise in the thermal functions due to crystallographic differences in the various crystalline samples.

Biler[1] [2] measured the heat capacity of B(cr, β) in the region 2–15 K. He reported $\theta_D = 1480$ K derived from his extrapolation to $T/K = 0$ of a graph of $(C_p - \gamma T)/T^3$ vs T^2. For boron, there is no electronic contribution, i.e. $\gamma = 0$. Only graphical data was presented. The sample, stated to be the β–rhombohedral modification based on X–ray data, contained 50 ppm Cu whereas the other impurities were reported as <1ppm (via electron micro–probe analysis).

Johnston *et al.*[3] measured 46 heat capacity values in the range 16.90–303.71 K. This study indicated a shallow maximum near 25 K at which ~~temperature~~ $C_p°$=0.038 $J{\cdot}K^{-1}{\cdot}mol^{-1}$. A graph of the results by Biler[1] [2] tends to agree with the observations of Johnston *et al.*[3] and to support the ~~presence of~~ a C_p anomaly. The purity of Johnston's sample was not reported. Hultgren *et al.*[8] stated that the sample was of the tetragonal (α) modification. This inference is presumably based on Johnston's reported method of preparation and X–ray data.

Bogdanov *et al.*[4] measured the heat capacity from 16 to 280 K. Metallic impurity content was stated to be <0.01 %. X–ray analysis was used to infer that the sample was the β–polymorph. Bogdanov *et al.* also inferred that the sample of Johnston *et al.* was not of a specific crystalline modification. They surmised that impurities caused the shallow maximum seen by Johnston *et al.*[3] near 25 K. Bogdanov *et al.* found no maximum, but their smooth values level out below 40 K in contradiction to theory. Their last five values (20–40 K) vary linearly with T and extrapolate to $C_p = 0.0126\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ at $T/K = 0$. The authors did not publish their experimental data, so it is difficult to interpret this behavior. It may arise from bias of their calorimeter near its limit of sensitivity or from anomalous behavior of their sample.

McDonald and Stull[5] measured enthalpies in a copper block drop calorimeter, 20 points in the range 282.8 to 1667.8 K. The sample was reported to be the β–rhombohedral form (based on X–ray data) with a metallic impurity of 0.59%. Stout *et al.*,[6] also using a copper block drop calorimeter, measured enthalpies, five data points in the range 1820–2218 K. The sample was reported to have 0.04% metallic impurities and to contain 300 ppm 0 and 6300 ppm C. No information as to crystalline form was given. Wise *et al.*[9] measured the enthalpy of two crystalline boron samples (each reportedly containing some of the β–modification) in the temperature range 515–1103 K.

The adopted heat capacity values below 25 K are derived from the θ_D value of Biler.[1] [2] From 25 K to 300 K, the derived values are a compromise of the data of Johnston *et al.*[3] and Bogdanov *et al.*,[4] but excluding in each the effect of the possible anomalous behavior. In the region 25 to 95 K, there is large scatter in each data set, so that large deviations occur, up to 23%. In the region 95–300 K, Johnston's data shows deviations of −2.1 to +1.8% while Bogdanov's data shows derviations of −2.9 to +1.7% from the adopted values. The two sets of data are intertwined, one is not always above the other.

In the enthalpy data, 26 of the 30 points of McDonald and Stull[5] are within +0.6% to −0.5%. Stout's[6] data deviates from −0.7% at 1819.5 K to +0.7% at 2217.7 K. The data of McDonald and Stull and Stout *et al.* are slightly skewed to each other. The observed enthalpies of McDonald and Stull[5] fall between the enthalpies of the two samples measured by Wise *et al.*[9]

Other heat capacity and enthalpy studies are available but were excluded from this analysis A detailed discussion of the Group IIIA metals (B, Al, and Ga) is in preparation by the JANAF staff.

Fusion Data

Refer to the liquid table for details.

Sublimation Data

The adopted value of $\Delta_{sub}H°(298.15\ K)$ is the value recommended by CODATA.[7] See the ideal gas table for details.

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Boron, Beta–Rhombohedral (B) $B_1(cr)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−1.214	0.	0.	0.
100	1.076	0.308	12.207	−1.190	0.	0.	0.
200	5.998	2.419	6.704	−0.857	0.	0.	0.
250	8.821	4.063	6.007	−0.486	0.	0.	0.
298.15	11.315	5.834	5.834	0.	0.	0.	0.
300	11.405	5.904	5.834	0.021	0.	0.	0.
350	13.654	7.834	5.981	0.648	0.	0.	0.
400	15.693	9.794	6.335	1.384	0.	0.	0.
450	17.361	11.742	6.828	2.211	0.	0.	0.
500	18.722	13.644	7.415	3.115	0.	0.	0.
600	20.778	17.251	8.758	5.096	0.	0.	0.
700	22.249	20.570	10.212	7.251	0.	0.	0.
800	23.361	23.617	11.699	9.534	0.	0.	0.
900	24.245	26.421	13.181	11.915	0.	0.	0.
1000	24.978	29.014	14.637	14.378	0.	0.	0.
1100	25.606	31.425	16.055	16.908	0.	0.	0.
1200	26.161	33.677	17.430	19.496	0.	0.	0.
1300	26.663	35.792	18.762	22.138	0.	0.	0.
1400	27.125	37.785	20.051	24.828	0.	0.	0.
1500	27.557	39.671	21.296	27.562	0.	0.	0.
1600	27.966	41.463	22.501	30.338	0.	0.	0.
1700	28.356	43.170	23.667	33.155	0.	0.	0.
1800	28.732	44.801	24.796	36.009	0.	0.	0.
1900	29.097	46.365	25.891	38.901	0.	0.	0.
2000	29.452	47.866	26.952	41.828	0.	0.	0.
2100	29.799	49.312	27.983	44.791	0.	0.	0.
2200	30.140	50.706	28.984	47.788	0.	0.	0.
2300	30.475	52.053	29.958	50.819	0.	0.	0.
2350.000	30.641	52.710	30.435	52.346	−−−− BETA <−−> LIQUID −−−−		
2400	30.806	53.357	30.906	53.883	−50.259	1.069	−0.023
2500	31.133	54.621	31.829	56.980	−50.337	3.209	−0.067
2600	31.457	55.848	32.730	60.109	−50.383	5.352	−0.108
2700	31.778	57.042	33.608	63.271	−50.396	7.496	−0.145
2800	32.096	58.203	34.466	66.465	−50.377	9.640	−0.180

PREVIOUS March 1979 CURRENT: June 1983

Boron, Beta–Rhombohedral (B) $B_1(cr)$

$S°(298.15\ K)$ = [26.555] J·K⁻¹·mol⁻¹
T_{fus} = 2350 ± 50 K

$\Delta_f H°(298.15\ K)$ = [48.927] kJ·mol⁻¹
$\Delta_{fus}H°$ = 50.2 ± 1.7 kJ·mol⁻¹

Enthalpy of Formation

The enthalpy of formation of liquid boron is calculated from that of the crystal (β–rhomohedral) by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(2350\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

There are no heat capacity or enthalpy studies which adequately define the liquid phase heat capacity values. Tsagareishvili and Tsagareishvili[1] estimated $C_p°(l)$ = 39.04 J·K⁻¹·mol⁻¹ at T_{fus} by means of quasi-thermodynamic correlations. Using our adopted $C_p°$ value for the crystal at T_{fus}, we recalculate this to be $C_p°(l)$ = 35.98 J·K⁻¹·mol⁻¹ at T_{fus}. This value appears to be too large. Even though B(cr) and Al(cr) have different crystal structures, the heat capacity values of the crystals at their respective T_{fus} are very similar, 30.64 J·K⁻¹·mol⁻¹ for B(β–cr) and 32.96 J·K⁻¹·mol⁻¹ for Al(cr). We estimate that the B(l) heat capacity is 31.75 J·K⁻¹·mol⁻¹, as is the value for Al(l).

A glass transition is assumed at 1760 K. The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

The adopted value for the melting point of β–rhombohedral boron is T_{fus} = 2350 ± 50 K. This value is within 2 K of the value recommended by Charlesworth.[2] The value is based primarily on the work of Kimpel and Moss.[3] These authors[3] used a disappearing hole technique to measure T_{fus} = 2352 ± 20 K for a 99.5% pure sample. Other studies are by Wisnyi and Pijanowski[4] (2313 ± 30 K), Cueilleron[5] (2273–2348 K), and Mar[6] (2315 ± 20 K).

The enthalpy of melting was measured by Stout et al.[7] using drop calorimetry. The enthalpy of melting, $\Delta_{fus}H°$ = 50.2 ± 1.7 kJ·mol⁻¹, was the result of three calorimetric determinations involving different samples and containers. It leads to an entropy of fusion, $\Delta_{fus}S°$ = 21.4 J·K⁻¹·mol⁻¹, which is more than twice as large as previous estimates.

Vaporization Data

There are no vaporization studies involving liquid boron The boiling point, T_{vap}(1 bar) = 4137.895 K, is calculated as the temperature for which $\Delta_f G°$=0 for B(l)=B(g). The difference in the enthalpy of formation of B(l) and B(g) at T_{vap} is the enthalpy of vaporization, $\Delta_{vap}H°$ = 480.344 kJ·mol⁻¹.

References

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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_f H°$ (kJ·mol⁻¹)	$\Delta_f G°$ (kJ·mol⁻¹)	log K_f
0							
100							
200							
250							
298.15	11.315	26.555	26.555	0.	48.927	42.749	−7.490
300	11.405	26.625	26.555	0.021	48.927	42.711	−7.437
350	13.654	28.554	26.702	0.648	48.927	41.675	−6.220
400	15.693	30.515	27.056	1.384	48.927	40.639	−5.307
450	17.361	32.463	27.549	2.211	48.927	39.603	−4.597
500	18.722	34.365	28.136	3.115	48.927	38.567	−4.029
600	20.778	37.971	29.479	5.096	48.927	36.495	−3.177
700	22.249	41.291	30.932	7.251	48.927	34.423	−2.569
800	23.361	44.337	32.420	9.534	48.927	32.351	−2.112
900	24.245	47.142	33.902	11.915	48.927	30.279	−1.757
1000	24.978	49.735	35.357	14.378	48.927	28.207	−1.473
1100	25.606	52.146	36.775	16.908	48.927	26.135	−1.241
1200	26.161	54.398	38.151	19.496	48.927	24.062	−1.047
1300	26.663	56.512	39.483	22.138	48.927	21.990	−0.884
1400	27.125	58.505	40.771	24.828	48.927	19.918	−0.743
1500	27.557	60.392	42.017	27.562	48.927	17.846	−0.621
1600	27.966	62.183	43.222	30.338	48.927	15.774	−0.515
1700	28.356	63.891	44.388	33.155	48.927	13.702	−0.421
1750.000	28.546	64.715	44.957	34.577	GLASS <--> LIQUID		
1750.000	31.750	64.715	44.957	34.577	TRANSITION		
1800	31.750	65.610	45.518	36.165	49.083	11.628	−0.337
1900	31.750	67.326	46 621	39.340	49.366	9.539	−0.262
2000	31.750	68.955	47.698	42.515	49.614	7.436	−0.194
2100	31.750	70.504	48.747	45.690	49.826	5.322	−0.132
2200	31.750	71.981	49.770	48.865	50.004	3.199	−0.076
2300	31.750	73.392	50.766	52.040	50.148	1.068	−0.024
2350.000	31.750	74.075	51.255	53.627	---- BETA <--> LIQUID ----		
2400	31.750	74.744	51.737	55.215	0.	0.	0.
2500	31.750	76.040	52.684	58.390	0.	0.	0.
2600	31.750	77.285	53.606	61.565	0.	0.	0.
2700	31.750	78.483	54.506	64.740	0.	0.	0.
2800	31.750	79.638	55.383	67.915	0.	0.	0.
2900	31.750	80.752	56.238	71.090	0.	0.	0.
3000	31.750	81.828	57.074	74.265	0.	0.	0.
3100	31.750	82.869	57.889	77.440	0.	0.	0.
3200	31.750	83.877	58.685	80.615	0.	0.	0.
3300	31.750	84.854	59.464	83.790	0.	0.	0.
3400	31.750	85.802	60.224	86.965	0.	0.	0.
3500	31.750	86.723	60.968	90.140	0.	0.	0.
3600	31.750	87.617	61.696	93.315	0.	0.	0.
3700	31 750	88.487	62.409	96.490	0.	0.	0.
3800	31.750	89.334	63.106	99.665	0.	0.	0.
3900	31.750	90.158	63.789	102.840	0.	0.	0.
4000	31.750	90.962	64.459	106.015	0.	0.	0.
4100	31.750	91.746	65.115	109.190	0.	0.	0.
4139.449	31.750	92.050	65.370	110.442	----- FUGACITY = 1 bar -----		
4200	31.750	92.511	65.758	112.365	−479.849	7.024	−0.087
4300	31.750	93.258	66.389	115.540	−478.762	18.603	−0.226
4400	31.750	93.988	67.008	118.715	−477.677	30.158	−0.358
4500	31.750	94.702	67.615	121.890	−476.593	41.687	−0.484

PREVIOUS: March 1979 CURRENT: June 1983

Boron (B) **CRYSTAL-LIQUID**

0 to 2350 K crystal
above 2350 K liquid

Refer to the individual tables for details.

$A_r = 10.81$ **Boron (B)** $B_1(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−1.214	0.	0.	0.
100	1.076	0.308	12.207	−1.190	0.	0.	0.
200	5.998	2.419	6.704	−0.857	0.	0.	0.
250	8.821	4.063	6.007	−0.486	0.	0.	0.
298.15	11.315	5.834	5.834	0.	0.	0.	0.
300	11.405	5.904	5.834	0.021	0.	0.	0.
350	13.654	7.834	5.981	0.648	0.	0.	0.
400	15.693	9.794	6.335	1.384	0.	0.	0.
450	17.361	11.742	6.828	2.211	0.	0.	0.
500	18.722	13.644	7.415	3.115	0.	0.	0.
600	20.778	17.251	8.758	5.096	0.	0.	0.
700	22.249	20.570	10.212	7.251	0.	0.	0.
800	23.361	23.617	11.699	9.534	0.	0.	0.
900	24.245	26.421	13.181	11.915	0.	0.	0.
1000	24.978	29.014	14.637	14.378	0.	0.	0.
1100	25.606	31.425	16.055	16.908	0.	0.	0.
1200	26.161	33.677	17.430	19.496	0.	0.	0.
1300	26.663	35.792	18.762	22.138	0.	0.	0.
1400	27.125	37.785	20.051	24.828	0.	0.	0.
1500	27.557	39.671	21.296	27.562	0.	0.	0.
1600	27.966	41.463	22.501	30.338	0.	0.	0.
1700	28.356	43.170	23.667	33.155	0.	0.	0.
1800	28.732	44.801	24.796	36.009	0.	0.	0.
1900	29.097	46.365	25.891	38.901	0.	0.	0.
2000	29.452	47.866	26.952	41.828	0.	0.	0.
2100	29.799	49.312	27.983	44.791	0.	0.	0.
2200	30.140	50.706	28.984	47.788	0.	0.	0.
2300	30.475	52.053	29.958	50.819	0.	0.	0.
2350.000	30.641	52.710	30.435	52.346	BETA <--> LIQUID TRANSITION		
2350.000	31.750	74.075	30.435	102.554			
2400	31.750	74.744	31.351	104.142	0.	0.	0.
2500	31.750	76.040	33.113	107.317	0.	0.	0.
2600	31.750	77.285	34.788	110.492	0.	0.	0.
2700	31.750	78.483	36.384	113.667	0.	0.	0.
2800	31.750	79.638	37.909	116.842	0.	0.	0.
2900	31.750	80.752	39.367	120.017	0.	0.	0.
3000	31 750	81.828	40.764	123.192	0.	0.	0.
3100	31.750	82.869	42.106	126.367	0.	0	0.
3200	31.750	83.877	43.396	129.542	0.	0.	0.
3300	31.750	84.854	44.637	132.717	0.	0.	0.
3400	31.750	85.802	45.834	135.892	0.	0.	0.
3500	31.750	86.723	46.989	139.067	0.	0.	0.
3600	31.750	87.617	48.105	142.242	0.	0.	0.
3700	31.750	88.487	49.185	145.417	0.	0.	0.
3800	31.750	89.334	50.231	148.592	0.	0.	0.
3900	31.750	90.158	51.244	151.767	0.	0.	0.
4000	31.750	90.962	52.227	154.942	0.	0.	0.
4100	31.750	91.746	53 181	158.117	0.	0.	0.
4139.449	31.750	92.050	53.550	159.369	----- FUGACITY = 1 bar -----		
4200	31.750	92.511	54.109	161.292	−479.849	7.024	−0.087
4300	31.750	93.258	55.010	164 467	−478.762	18.604	−0.226
4400	31.750	93.988	55.888	167.642	−477.677	30.158	−0.358
4500	31.750	94.702	56.743	170.817	−476.593	41.687	−0.484

PREVIOUS: March 1979 CURRENT June 1983

Boron (B) $B_1(cr,l)$

Boron (B) IDEAL GAS $A_r = 10.81$ Boron (B) $B_1(g)$

IP(B, g) = 66928.10 ± 1 cm^{-1}
$S°(298.15\ K)$ = 153.435 ± 0.035 J·K^{-1}·mol^{-1}

$\Delta_f H°(0\ K)$ = 555 ± 12 kJ·mol^{-1}
$\Delta_f H°(298.15\ K)$ = 560 ± 12 kJ·mol^{-1}

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2P°_{1/2}$	0.00	2
$^2P°_{3/2}$	15.254	4
$^4P_{1/2}$	28870.0	2
.	.	.
.	.	.
.	.	.
$^2D_{5/2}$	66855.78	6
IP	66928.10	

Enthalpy of Formation

The enthalpy of formation is derived from the measurements of Paule and Margrave,[1] Robson and Gilles,[2] Hildenbrand and Hall,[3] Akishin *et al.*,[4] and Schissel and Trulson.[5] $\Delta_f H°(B, g, 298.15\ K)$ = 560 ± 12 kJ·mol^{-1} is the value recommended by CODATA.[6] CODATA stated that these measurements were selected from the many sets of data available as being the most self-consistent. The difference in $S°(B, cr, 298.15\ K)$ between our adopted value and that of CODATA,[6] will create a change of less than 0.2 kJ·mol^{-1} in $\Delta_f H°(B, g, 298.15\ K)$. Not included in this analysis are other vaporization studies by Trulson *et al.* (1923–2249 K),[7] Burns *et al.* (2403 K),[8] Mar and Bedford (1823–2253 K),[9] and Storms and Mueller (1750–2050 K).[10] The two latter studies were published after the time of the CODATA analysis. Inclusion of these studies would suggest a somewhat larger value for $\Delta_f H$. The $\Delta_f H°(B, g, 298.15\ K)$ values reported by Mar and Bedford[9] are 563.6 ± 33.4 kJ·mol^{-1} (2nd law) and 561.1 ± 3.3 kJ·mol^{-1} (3rd law) from torsion data and 566.1 ± 13.3 kJ·mol^{-1} from mass spectrometric data; Storms and Mueller[10] reported 574.9 ± 0.8 kJ·mol^{-1} as the 2nd law value derived from a mass spectrometric study.

Heat Capacity and Entropy

The electronic levels are from the recent analysis by Odintzova and Striganov.[11] Although only the ground state, first two excited states, and the highest observed state (below the ionization limit) are listed, all reported states below the ionization limit are used in the calculations. The 164 observed levels are too numerous to list completely, but do include contributions from observed levels to n=39.

The level at 15.254 cm^{-1} has a large effect on the heat capacity and entropy below 100 K. The heat capacity effect decreases to zero above 600 K where the 15.254 cm^{-1} level is fully populated. The higher excited states affect the heat capacity values above 3000 K. The Gibbs energy function values up to 6000 K are essentially independent of the cut-off procedure, the inclusion of levels for $n>2$, and the estimated missing levels (for n<39).

The thermal functions at 298.15 K agree with recent CODATA recommendations[1] except for two minor differences. First, the entropy differs by 0.1094 J·K^{-1}·mol^{-1} because this table uses a standard state pressure of 1 bar, whereas the CODATA recommendations are based on 1 atm. Second, an entropy difference of 0.001 J·K^{-1}·mol^{-1} arises due to the use of slightly different values for the fundamental constants.

References

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.316	554.898	554.898	INFINITE
100	20.881	130.687	171.936	−4.125	557.065	544.027	−284.171
200	20.809	145.130	155.338	−2.042	558.815	530.273	−138.493
250	20.801	149.772	153.778	−1.001	559.485	523.057	−109.287
298.15	20.796	153.435	153.435	0.	560.000	515.993	−90.400
300	20.796	153.564	153.436	0.038	560.017	515.720	−89.795
350	20.793	156.769	153.689	1.078	560.430	508.302	−75.860
400	20.792	159.546	154.251	2.118	560.734	500.834	−65.402
450	20.790	161.995	154.978	3.157	560.946	493.332	−57.265
500	20.790	164.185	155.791	4.197	561.082	485.812	−50.752
600	20.789	167.975	157.516	6.276	561.180	470.745	−40.982
700	20.788	171.180	159.245	8.355	561.104	455.677	−34.003
800	20.787	173.956	160.914	10.433	560.900	440.628	−28.770
900	20.787	176.404	162.502	12.512	560.597	425.612	−24.702
1000	20.787	178.594	164.003	14.591	560.213	410.633	−21.449
1100	20.787	180.575	165.421	16.669	559.762	395.697	−18.790
1200	20.787	182.384	166.761	18.748	559.252	380.804	−16.576
1300	20.787	184.048	168.027	20.827	558.689	365.955	−14.704
1400	20.786	185.588	169.227	22.905	558.078	351.152	−13.102
1500	20.786	187.023	170.366	24.984	557.422	336.395	−11.714
1600	20.786	188.364	171.450	27.063	556.724	321.682	−10.502
1700	20.786	189.624	172.482	29.141	555.987	307.014	−9.433
1800	20.786	190.812	173.468	31.220	555.211	292.391	−8.485
1900	20.786	191.936	174.411	33.299	554.398	277.812	−7.638
2000	20.786	193.002	175.314	35.377	553.549	263.277	−6.876
2100	20.786	194.017	176.180	37.456	552.665	248.785	−6.188
2200	20.786	194.984	177.013	39.535	551.747	234.335	−5.564
2300	20.786	195.908	177.815	41.613	550.795	219.929	−4.995
2400	20.786	196.792	178.587	43.692	499.550	206.633	−4.497
2500	20.786	197.641	179.333	45.770	498.453	194.451	−4.063
2600	20.787	198.456	180.052	47.849	497.357	182.312	−3.663
2700	20.787	199.240	180.749	49.928	496.261	170.216	−3.293
2800	20.787	199.996	181.423	52.006	495.165	158.160	−2.951
2900	20.788	200.726	182.076	54.085	494.068	146.144	−2.632
3000	20.789	201.431	182.709	56.164	492.972	134.165	−2.336
3100	20.791	202.112	183.324	58.243	491.876	122.223	−2.059
3200	20.793	202.772	183.922	60.322	490.780	110.316	−1.801
3300	20.795	203.412	184.503	62.402	489.685	98.444	−1.558
3400	20.798	204.033	185.068	64.481	488.589	86.604	−1.331
3500	20.803	204.636	185.619	66.561	487.494	74.797	−1.116
3600	20.808	205.222	186.155	68.642	486.400	63.021	−0.914
3700	20.814	205.792	186.678	70.723	485.306	51.276	−0.724
3800	20.822	206.348	187.188	72.805	484.213	39.560	−0.544
3900	20.831	206.889	187.687	74.887	483.120	27.873	−0.373
4000	20.842	207.416	188.173	76.971	482.029	16.214	−0.212
4100	20.855	207.931	188.649	79.056	480.939	4.582	−0.058
4139.449	20.860	208.131	188.834	79.879	----- FUGACITY = 1 bar -----		
4200	20.870	208.434	189.114	81.142	0.	0.	0.
4300	20.887	208.925	189.569	83.230	0.	0.	0.
4400	20.906	209.405	190.015	85.319	0.	0.	0.
4500	20.928	209.875	190.451	87.411	0.	0.	0.
4600	20.952	210.336	190.878	89.505	0.	0.	0.
4700	20.979	210.786	191.297	91.602	0.	0.	0.
4800	21.009	211.228	191.707	93.701	0.	0.	0.
4900	21.042	211.662	192.110	95.803	0.	0.	0.
5000	21.078	212.087	192.506	97.909	0.	0.	0.
5100	21.117	212.505	192.894	100.019	0.	0.	0.
5200	21.160	212.916	193.275	102.133	0.	0.	0.
5300	21.206	213.319	193.649	104.251	0.	0.	0.
5400	21.255	213.716	194.017	106.374	0.	0.	0.
5500	21.308	214.107	194.379	108.502	0.	0.	0.
5600	21.365	214.491	194.735	110.636	0.	0.	0.
5700	21.425	214.870	195.084	112.776	0.	0.	0.
5800	21.489	215.243	195.429	114.921	0.	0.	0.
5900	21.557	215.611	195.768	117.073	0.	0.	0.
6000	21.628	215.974	196.101	119.233	0.	0.	0.

PREVIOUS. March 1979 (1 atm)   CURRENT June 1983 (1 bar)

Boron, Ion (B^+) IDEAL GAS $M_r = 10.80945$ Boron, Ion (B^+) $B^+_1(g)$

IP(B^+, g) = 202887.4 ± 0.8 cm^{-1}
$S°$(298.15 K) = 138.542 ± 0.04 $J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°$(0 K) = 1356 ± 12 $kJ{\cdot}mol^{-1}$
$\Delta_f H°$(298.15 K) = [1366.717] $kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights State	ϵ_i, cm^{-1}	g_i
$^2S_0$	0.0	1
$^3P_0$	37333.6	1
$^3P_1$	37340.0	3
$^3P_2$	37356.4	5

Enthalpy of Formation

$\Delta_f H°$(B^+, g, 0 K) is calculated from $\Delta_f H°$(B, g, 0 K)[1] using the spectroscopic value of IP(B) = 66928.10 ± 0.1 cm^{-1} (800.638 ± 0.001 $kJ{\cdot}mol^{-1}$) from Odintzova and Striganov.[2] The ionization limit is converted from cm^{-1} to $kJ{\cdot}mol^{-1}$ using the factor, 1 cm^{-1} = 0.01196266 $kJ{\cdot}mol^{-1}$, which is derived from the 1973 CODATA fundamental constants.[3] Rosenstock *et al.*[4] and Levin and Lias[5] have summarized additional ionization and appearance potential data.

$\Delta_f H°$(B^+, g, 298.15 K) is calculated from $\Delta_f H°$(B, g, 0 K) by using IP(B) with JANAF[1] enthalpies, $H°$(0 K)–$H°$(298.15 K), for B(g), B^+(g), and e^-(ref). $\Delta_f H°$($B \rightarrow B^+ + e^-$, 298.15 K) differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[4] $\Delta_f H°$(298.15 K) should be changed by −6.197 $kJ{\cdot}mol^{-1}$ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Moore,[6,7] 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[8] 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 three excited states; the next excited state is 73396.7 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 and the first three excited states. The energies of the ^3P levels are uncertain by 249 cm^{-1}. No intersystem combinations have been observed. The reported uncertainty in $S°$(298.15 K) is due to uncertainties in the relative ionic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the excited states and use of different fill and cutoff procedures.[8]

Refereces

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	-6.197	1355.536		
100	20.786	115.835	157.023	-4.119			
200	20.786	130.243	140.444	-2.040			
250	20.786	134.881	138.885	-1.001			
298.15	20.786	138.542	138.542	0.	1366.717	1320.895	-231.415
300	20.786	138.671	138.543	0.038	1366.773	1320.611	-229.939
350	20.786	141.875	138.796	1.078	1368.224	1312.801	-195.925
400	20.786	144.651	139.358	2.117	1369.567	1304.790	-170.388
450	20.786	147.099	140.085	3.156	1370.818	1296.617	-150.507
500	20.786	149.289	140.898	4.196	1371.994	1288.309	-134.589
600	20.786	153.079	142.622	6.274	1374.170	1271.364	-110.682
700	20.786	156.283	144.350	8.353	1376.172	1254.069	-93.580
800	20.786	159.058	146.019	10.431	1378.046	1236.497	-80.735
900	20.786	161.507	147.607	12.510	1379.822	1218.696	-70.731
1000	20.786	163.697	149.108	14.589	1381.517	1200.701	-62.718
1100	20.786	165.678	150.526	16.667	1383.144	1182.540	-56.154
1200	20.786	167.486	151.865	18.746	1384.712	1164.234	-50.678
1300	20.786	169.150	153.131	20.824	1386.228	1145.799	-46.039
1400	20.786	170.691	154.331	22.903	1387.695	1127.249	-42.058
1500	20.786	172.125	155.470	24.982	1389.118	1108.596	-38.605
1600	20.786	173.466	156.553	27.060	1390.499	1089.849	-35.580
1700	20.786	174.726	157.586	29.139	1391.840	1071.017	-32.908
1800	20.786	175.914	158.571	31.217	1393.143	1052.108	-30.531
1900	20.786	177.038	159.514	33.296	1394.408	1033.127	-28.403
2000	20.786	178.104	160.417	35.375	1395.638	1014.080	-26.485
2100	20.786	179.119	161.284	37.453	1396.833	994.972	-24.749
2200	20.786	180.086	162.117	39.532	1397.993	975.809	-23.169
2300	20.786	181.010	162.918	41.610	1399.119	956.593	-21.725
2400	20.786	181.894	163.690	43.689	1349.953	938.398	-20.424
2500	20.786	182.743	164.436	45.768	1350.935	921.230	-19.248
2600	20.786	183.558	165.156	47.846	1351.917	904.023	-18.162
2700	20.786	184.342	165.852	49.925	1352.900	886.777	-17.156
2800	20.786	185.098	166.526	52.004	1353.882	869.495	-16.221
2900	20.786	185.828	167.179	54.082	1354.864	852.179	-15.349
3000	20.786	186.532	167.812	56.161	1355.846	834.828	-14.536
3100	20.787	187.214	168.427	58.239	1356.829	817.444	-13.774
3200	20.787	187.874	169.025	60.318	1357.811	800.029	-13.059
3300	20.788	188.514	169.606	62.397	1358.793	782.583	-12.387
3400	20.789	189.134	170.171	64.476	1359.776	765.108	-11.754
3500	20.790	189.737	170.721	66.555	1360.758	747.603	-11.157
3600	20.792	190.323	171.258	68.634	1361.741	730.070	-10.593
3700	20.794	190.892	171.781	70.713	1362.724	712.511	-10.059
3800	20.797	191.447	172.291	72.792	1363.707	694.924	-9.552
3900	20.801	191.987	172.789	74.872	1364.690	677.312	-9.072
4000	20.806	192.514	173.276	76.953	1365.674	659.674	-8.614
4100	20.812	193.028	173.751	79.034	1366.659	642.012	-8 179
4200	20.820	193.529	174.216	81.115	887.795	631.350	-7.852
4300	20.830	194.019	174.671	83.198	889.868	625.219	-7.595
4400	20.841	194.498	175.116	85.281	891.940	619.041	-7.349
4500	20.856	194.967	175.552	87.366	894.012	612.815	-7.113
4600	20.872	195.425	175.979	89.452	896.083	606.544	-6.888
4700	20.892	195.874	176.398	91.540	898.153	600.227	-6.671
4800	20.915	196.314	176.808	93.631	900.223	593.866	-6.463
4900	20.941	196.746	177.211	95.724	902.292	587.462	-6.262
5000	20.972	197.169	177.606	97.819	904.360	581.016	-6.070
5100	21.006	197.585	177.993	99.918	906.428	574.529	-5.884
5200	21.046	197.993	178.374	102.021	908.495	568.001	-5.706
5300	21.090	198.395	178.748	104.127	910.562	561.433	-5.533
5400	21.139	198.789	179.115	106.239	912.629	554.827	-5.367
5500	21.194	199.178	179.477	108.355	914.696	548.182	-5.206
5600	21.254	199.560	179.832	110.478	916.764	541.499	-5.051
5700	21.321	199.937	180.181	112.606	918.831	534.779	-4.901
5800	21.393	200.308	180.525	114.742	920.900	528.024	-4.755
5900	21.473	200.675	180.864	116.885	922.970	521.232	-4.615
6000	21.558	201.036	181.197	119.037	925.040	514.406	-4.478

PREVIOUS: March 1979 (1 atm) CURRENT: June 1983 (1 bar)

Boron, Ion (B^-) IDEAL GAS $M_r = 10.81055$ Boron, Ion (B^-) $B_1^-(g)$

EA(B, g) = 0.277 ± 0.010 eV
$S°(298.15\ K) = 156.811 \pm 0.005\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 528 \pm 12\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = [527.033]\ kJ{\cdot}mol^{-1}$

Electonic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^3P_0$	0.0	1
$^3P_1$	4.0	3
$^3P_2$	9.0	5

Enthalpy of Formation

$\Delta_fH°(B^-, g, 0\ K)$ is calculated from $\Delta_fH°(B, g, 0\ K)$[1] using the adopted election affinity of EA(B) = 0.277 ± 0.010 eV (26.726 ± 0.965 $kJ{\cdot}mol^{-1}$). This value, recommended by Hotop and Lineberger[2] is based on a laser photodetachment electron spectrometry study.[3] Additional information on $B^-(g)$ may be obtained in the critical discussions of Hotop and Lineberger,[2,4] Rosenstock *et al.*[5] and Massey.[6]

$\Delta_fH°(B^-, g, 298.15\ K)$ is obtained from $\Delta_fH°(B, g, 0\ K)$ by using EA(B) with JANAF [1]enthalpies, $H°(0\ K)-H°(298.15\ K)$, for $B^-(g)$, B(g), and e^-(ref). $\Delta_rH°(B^- \rightarrow B + e^-, 298.15\ K)$ differs from a room–temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[5] $\Delta_fH°(298.15\ K)$ should be changed by +6.197 $kJ{\cdot}mol^{-1}$ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The ground state electronic configuration for $B^-(g)$ is given by Hotop and Lineberger,[2,4] Rosenstock *et al.*[5] and Massey.[6] The fine–structure separation has been calculated via an isoelectronic extrapolation of ratios of fine structure separations[4] and is that recommended by Hotop and Lineberger.[2]

A comparison of the isoelectronic sequence $B^-(g)$, C(g), $N^+(g)$, $O^{++}(g)$ would suggest that a state, $^1D_2$, may exist at low energy, 5000 cm^{-1}. However, this is most likely a metastable state lying at an energy greater than the electron affinity. As discussed by Hotop and Lineberger,[2,4] no stable excited states have been observed. Thus we assume no stable excited states exist.

References

[1] JANAF Thermochemical Tables: B(g), 6–30–83, e^-(ref), 3–31–82.
[2] H. Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data, 14, 731, (1985).
[3] C. S. Feigerle, R. R. Corderman and W. C. Lineberger, J. Chem. Phys. 74, 1513 (1981).
[4] H. Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data 4, 539 (1975).
[5] H. M. Rosenstock, K. Draxl *et al.*, J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).
[6] H. S. W. Massey, "Negative Ions", 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−6.273	528.172		
100	20.804	134.096	175.295	−4.120			
200	20.790	148.511	158.713	−2.040			
250	20.789	153.150	157.153	−1.001			
298.15	20.788	156.811	156.811	0.	527.033	488.274	−85.544
300	20.788	156.940	156.812	0.038	527.012	488.034	−84.974
350	20.787	160.144	157.065	1.078	526.385	481.585	−71.873
400	20.787	162.920	157.627	2.117	525.650	475.234	−62.059
450	20.787	165.368	158.354	3.157	524.822	468.981	−54.438
500	20.787	167.558	159.167	4.196	523.919	462.824	−48.351
600	20.787	171.348	160.891	6.275	521.938	450.788	−39.245
700	20.786	174.553	162.619	8.353	519.783	439.098	−32.766
800	20.786	177.328	164.288	10.432	517.500	427.726	−27.928
900	20.786	179.776	165.876	12.510	515.118	416.647	−24.182
1000	20.786	181.966	167.377	14.589	512.656	405.837	−21.199
1100	20.786	183.948	168.795	16.668	510.126	395.277	−18.770
1200	20.786	185.756	170.134	18.746	507.537	384.950	−16.756
1300	20.786	187.420	171.401	20.825	504.896	374.841	−15.061
1400	20.786	188.960	172.601	22.904	502.206	364.938	−13.616
1500	20.786	190.395	173.740	24.982	499.472	355.228	−12.370
1600	20.786	191.736	174.823	27.061	496 695	345.702	−11.286
1700	20.786	192.996	175.855	29.139	493.879	336.351	−10.335
1800	20.786	194.184	176.841	31.218	491.025	327.167	−9.494
1900	20.786	195.308	177.784	33.297	488.133	318.142	−8.746
2000	20.786	196.374	178.687	35.375	485.206	309.271	−8.077
2100	20.786	197.388	179.553	37.454	482.243	300.547	−7.476
2200	20.786	198.355	180.386	39.532	479.246	291.965	−6.932
2300	20.786	199.279	181.188	41.611	476.215	283.520	−6.439
2400	20.786	200.164	181.960	43.690	422.892	276.276	−6.013
2500	20.786	201.013	182.705	45.768	419.717	270.232	−5.646
2600	20.786	201.828	183.425	47.847	416.542	264.315	−5.310
2700	20.786	202.612	184.121	49.925	413.367	258.521	−5.001
2800	20.786	203.368	184.795	52.004	410.192	252.844	−4.717
2900	20.786	204.098	185.448	54.083	407.017	247.280	−4.454
3000	20.786	204.802	186.082	56.161	403.842	241.826	−4.211
3100	20.786	205.484	186.697	58.240	400.667	236.478	−3.985
3200	20.786	206.144	187.294	60.318	397.492	231.232	−3.774
3300	20.786	206.783	187.875	62.397	394.317	226.086	−3.579
3400	20.786	207.404	188.441	64.476	391.142	221.036	−3.396
3500	20.786	208.007	188.991	66.554	387.967	216.079	−3.225
3600	20.786	208.592	189.527	68.633	384.792	211.213	−3.065
3700	20.786	209.162	190.050	70.711	381.617	206.435	−2.914
3800	20.786	209 716	190.561	72.790	378.442	201.743	−2.773
3900	20.786	210.256	191.059	74.869	375.267	197.134	−2.640
4000	20.786	210.782	191.545	76.947	372.092	192.607	−2.515
4100	20.786	211.295	192.021	79.026	368.917	188.159	−2.397
4200	20.786	211.796	192.486	81.104	−114.108	190.813	−2.373
4300	20.786	212.285	192.940	83.183	−116.195	198.097	−2.406
4400	20.786	212.763	193.386	85.262	−118.285	205.431	−2.439
4500	20.786	213.230	193.821	87.340	−120.377	212.811	−2.470
4600	20.786	213.687	194.248	89.419	−122.471	220.239	−2.501
4700	20.786	214.134	194.667	91.498	−124.567	227.712	−2.531
4800	20.786	214.572	195.077	93.576	−126.666	235.229	−2.560
4900	20.786	215.000	195.479	95.655	−128.769	242.790	−2.588
5000	20.786	215.420	195.874	97.733	−130.875	250.395	−2.616
5100	20.786	215.832	196.261	99.812	−132.985	258.041	−2.643
5200	20.786	216.236	196.641	101.891	−135.099	265.729	−2.669
5300	20.786	216.632	197.015	103.969	−137.217	273.457	−2.695
5400	20.786	217.020	197.382	106.048	−139.340	281.225	−2.720
5500	20.786	217.401	197.742	108.126	−141.468	289.033	−2.745
5600	20.786	217.776	198.097	110.205	−143.602	296.880	−2.769
5700	20.786	218.144	198.445	112.284	−145.741	304.765	−2.793
5800	20.786	218.505	198.788	114.362	−147.887	312.687	−2.816
5900	20.786	218.861	199.125	116.441	−150.039	320.646	−2.839
6000	20.786	219.210	199.457	118.519	−152.198	328.642	−2.861

PREVIOUS: March 1979 (1 atm) CURRENT: June 1983 (1 bar)

Beryllium Borate (BeBO$_2$) IDEAL GAS M_r = 51.82098 Beryllium Borate (BeBO$_2$) B$_1$Be$_1$O$_2$(g)

$S°(298.15 \text{ K}) = [265.4] \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = -481.8 \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = -482.0 \text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}	υ, cm^{-1}
[2000](1)	[600](1)
[1000](1)	[400](1)
[900](1)	[800](1)

Ground State Quantum Weight: [2] σ = [1]
Point Group: [C$_s$]
Bond Distances: Be–O = [1.40] Å; O–B = [1.36] Å; B=O = [1.20] Å
Bond Angles: Be–O–B = [120]°; O–B = [180]°
Product of the Moments of Inertia: $I_A I_B I_C = [2.451196 \times 10^{-115}] \text{ g}^3\text{·cm}^6$

Enthalpy of Formation

Since Blackburn and Buchler[1] have postulated that the BO_2^- group has the pseudochloride character in bond strength, the enthalpy of formation of BeBO$_2$(g) is estimated by adding the difference of the enthalpies of formation of BeCl(g) and AlCl(g) to the enthalpies of formation of AlBO$_2$(g), using all JANAF values: $\Delta_f H°$(BeCl, g, 298.15 K) = 3.0, $\Delta_f H°$(AlCl, g, 298.15 K) = −11.2 and $\Delta_f H°$(AlBO$_2$, g, 298.15 K) = −129.4 kcal·mol^{-1}.

Heat Capacity and Entropy

All molecular constants are estimated by comparison with those in LiBO$_2$(g), AlBO$_2$(g), B$_2$O$_3$(g) and BeCl(g). The principal moments of inertia are $I_A = 1.1016 \times 10^{-39}$, $I_B = 14.3762 \times 10^{-39}$ and $I_C = 15.4778 \times 10^{-39}$ g·cm^2.

Reference

[1] P. E. Blackburn and A. Buchler, J. Phys. Chem. 69, 4250 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.594	−481.761	−481.761	INFINITE
100	34.261	221.501	304.015	−8.251	−481.387	−486.125	253.926
200	41.473	247.191	269.710	−4.504	−481.461	−490.883	128.206
250	46.006	256.932	266.199	−2.317	−481.694	−493.214	103.051
298.15	50.168	265.396	265.396	0.	−481.997	−495.406	86.793
300	50.320	265.707	265.397	0.093	−482.010	−495.489	86.272
350	54.165	273.759	266.024	2.707	−482.377	−497.707	74.279
400	57.492	281.215	267.463	5.501	−482.778	−499.870	65.276
450	60.347	288.155	269.381	8.449	−483.201	−501.982	58.269
500	62.797	294.644	271.586	11.529	−483.642	−504.045	52.657
600	66.738	306.459	276.434	18.015	−484.564	−508.040	44.229
700	69.721	316.981	281.488	24.845	−485.535	−511.876	38.197
800	72.017	326.447	286.527	31.936	−486.560	−515.570	33.663
900	73.810	335.037	291.447	39.231	−487.645	−519.132	30.130
1000	75.228	342.890	296.204	46.686	−488.797	−522.569	27.296
1100	76.363	350.115	300.781	54.267	−490.026	−525.888	24.972
1200	77.282	356.800	305.174	61.951	−491.338	−529.091	23.031
1300	78.033	363.017	309.387	69.718	−492.741	−532.180	21.383
1400	78.655	368.823	313.428	77.554	−494.241	−535.159	19.967
1500	79.173	374.268	317.304	85.446	−495.845	−538.026	18.736
1600	79.609	379.392	321.026	93.385	−512.094	−540.257	17.638
1700	79.978	384.230	324.603	101.365	−513.520	−541.974	16.653
1800	80.295	388.810	328.044	109.379	−514.997	−543.606	15.775
1900	80.567	393.159	331.358	117.423	−516.525	−545.154	14.987
2000	80.802	397.298	334.552	125.491	−518.109	−546.620	14.276
2100	81.007	401.245	337.635	133.582	−519.751	−548.005	13.631
2200	81.187	405.018	340.612	141.692	−521.452	−549.310	13.042
2300	81.346	408.630	343.492	149.819	−523.213	−550.538	12.503
2400	81.486	412.095	346.278	157.961	−575.297	−550.618	11.984
2500	81.611	415.424	348.978	166.116	−577.262	−549.550	11.482
2600	81.722	418.627	351.596	174.282	−579.258	−548.402	11.018
2700	81.822	421.714	354.136	182.460	−581.286	−547.177	10.586
2800	81.911	424.691	356.603	190.646	−874.304	−539.653	10.067
2900	81.992	427.567	359.001	198.842	−875.334	−527.684	9.505
3000	82.066	430.348	361.333	207.045	−876.380	−515.678	8.979
3100	82.132	433.040	363.603	215.255	−877.445	−503.636	8.486
3200	82.193	435.648	365.814	223.471	−878.529	−491.561	8.024
3300	82.248	438.178	367.968	231.693	−879.634	−479.452	7.589
3400	82.299	440.634	370.070	239.920	−880.761	−467.308	7.179
3500	82.346	443.021	372.120	248.153	−881.911	−455.131	6.792
3600	82.388	445.341	374.122	256.389	−883.088	−442.921	6.427
3700	82.428	447.599	376.077	264.630	−884.291	−430.678	6.080
3800	82.464	449.798	377.988	272.875	−885.524	−418.400	5.751
3900	82.498	451.940	379.857	281.123	−886.788	−406.091	5.439
4000	82.530	454.029	381.686	289.374	−888.085	−393.750	5.142
4100	82.559	456.067	383.475	297.629	−889.417	−381.375	4.859
4200	82.586	458.057	385.227	305.886	−1370.635	−361.943	4.501
4300	82.611	460.001	386.944	314.146	−1370.957	−337.922	4.105
4400	82.635	461.900	388.626	322.408	−1371.321	−313.895	3.726
4500	82.657	463.758	390.275	330.673	−1371.730	−289.858	3.365
4600	82.678	465.575	391.892	338.940	−1372.188	−265.812	3.018
4700	82.697	467.353	393.479	347.208	−1372.695	−241.754	2.687
4800	82.715	469.094	395.036	355.479	−1373.255	−217.686	2.369
4900	82.732	470.800	396.565	363.751	−1373.870	−193.605	2.064
5000	82.748	472.471	398.066	372.025	−1374.542	−169.511	1.771
5100	82.764	474.110	399.541	380.301	−1375.272	−145.403	1.489
5200	82.778	475.717	400.991	388.578	−1376.064	−121.281	1.218
5300	82.792	477.294	402.416	396.857	−1376.919	−97.142	0.957
5400	82.804	478.842	403.817	405.136	−1377.840	−72.987	0.706
5500	82.817	480.361	405.195	413.417	−1378.827	−48.815	0.464
5600	82.828	481.854	406.550	421.700	−1379.883	−24.622	0.230
5700	82.839	483.320	407.884	429.983	−1381.010	−0.412	0.004
5800	82.849	484.761	409.197	438.267	−1382.209	23.820	−0.215
5900	82.859	486.177	410.490	446.553	−1383.481	48.071	−0.426
6000	82.868	487.570	411.763	454.839	−1384.829	72.347	−0.630

PREVIOUS: June 1966 (1 atm)   CURRENT. June 1966 (1 bar)

Bromoborane (BBr) IDEAL GAS $M_r = 90.714$ Bromoborane (BBr) $B_1Br_1(g)$

$\Delta_f H°(0\ K) = 239 \pm 42\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 234 \pm 42\ kJ{\cdot}mol^{-1}$

$S°(298.15\ K) = 225.00\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

Electronic Level and Quantum Weight State	ϵ_i, cm^{-1}	g_i
$^1\Sigma^+$	0	1

$\omega_e = 689.04\ cm^{-1}$ $\omega_e x_e = 3.57\ cm^{-1}$ $\sigma = 1$
$B_e = 0.497\ cm^{-1}$ $\alpha_e = 0.0036\ cm^{-1}$ $r_e = 1.887\ Å$

Enthalpy of Formation

Herzberg[1] reported $D_0^\circ = 4.1$ eV which corresponds to a enthalpy of formation of 64 $kcal{\cdot}mol^{-1}$. Gaydon[2] gives essentially the same value, with a provisor that the value is unreliable due to the ionic nature of the bonding. Barrow[3] made a critical evaluation of the bond dissociation energies of the group III halides and concluded $D_0^\circ(BBr) = 103.5$ which gives $\Delta_f H°(298.15\ K) = 56\ kcal{\cdot}mol^{-1}$. An estimate of the dissociation energy by taking the ratio $D_0^\circ(BF)/[\Delta_a H°(BF_3, g, 0\ K)/3] = 1\ 177$ and applying this to BBr_3 yields $D_0^\circ(BBr) = 103\ kcal{\cdot}mol^{-1}$; this was the value adopted.

Heat Capacity and Entropy

The vibrational and rotational constants are all taken from NBS.[4]

References

[1] G. Herzberg, "Molecular Spectra and Molecular Structure of Diatomic Molecules," 2nd ed., D. van Nostrand Co., New York, 658 pp. (1950) refer to p. 506.

[2] A. G. Gaydon, "Dissociation Energies and Spectra of Diatomic Molecules," 2nd ed., Chapman and Hall, London, 261 pp. (1953).

[3] R. F. Barrow, Trans. Faraday Soc. 56, 952 (1960).

[4] U. S. Nat. Bur. Stand. Report 7093, 255 pp. (1962).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	-8.997	238.775	238.775	INFINITE
100	29.154	191.806	252.688	-6.088	240.264	223.806	-116.904
200	30.637	212.350	227.930	-3.116	240.453	207.208	-54.117
250	31.784	219.311	225.531	-1.555	240.234	198.918	-41.562
298.15	32.788	224.997	224.997	0.	234.304	191.651	-33.576
300	32.824	225.200	224.998	0.061	234.274	191.386	-33.323
350	33.684	230.327	225.400	1.724	218.985	185.073	-27.621
400	34.373	234.871	226.306	3.426	219.037	180.225	-23.535
450	34.921	238.953	227.488	5.159	219.021	175.373	-20.357
500	35.359	242.656	228.822	6.917	218.950	170.527	-17.815
600	35.999	249.163	231.685	10.487	218.679	160.865	-14.005
700	36.435	254.747	234.590	14.110	218.278	151.260	-11.287
800	36.747	259.633	237.422	17.770	217.779	141.719	-9.253
900	36.981	263.976	240.135	21.456	217.202	132.245	-7.675
1000	37.164	267.882	242.718	25.164	216.560	122.839	-6.416
1100	37.311	271.431	245.169	28.888	215.863	113.500	-5.390
1200	37.434	274.683	247.495	32.626	215.116	104.227	-4.537
1300	37.539	277.684	249.703	36.374	214.322	95.019	-3.818
1400	37.631	280.469	251.803	40.133	213.487	85.872	-3.204
1500	37.714	283.068	253.801	43.900	212.610	76.787	-2.674
1600	37.788	285.505	255.707	47.675	211.694	67.762	-2.212
1700	37.857	287.798	257.528	51.458	210.740	58.796	-1.807
1800	37.921	289.963	259.271	55.247	209.747	49.886	-1.448
1900	37.982	292.015	260.941	59.042	208.717	41.033	-1.128
2000	38.039	293.965	262.543	62.843	207.647	32.235	-0.842
2100	38.094	295.822	264.084	66.650	206.540	23.491	-0.584
2200	38.147	297.596	265.568	70.462	205.393	14.801	-0.351
2300	38.199	299.292	266.997	74.279	204.207	6.165	-0.140
2400	38.249	300.919	268.377	78.101	152.722	-1.351	0.029
2500	38.297	302.482	269.710	81.929	151.379	-7.743	0.162
2600	38.345	303.985	271.000	85.761	150.029	-14.081	0.283
2700	38.392	305.433	272.248	89.598	148.674	-20.368	0.394
2800	38.438	306.830	273.459	93.439	147.312	-26.604	0.496
2900	38.483	308.179	274.633	97.285	145.944	-32.791	0.591
3000	38.528	309.485	275.773	101.136	144.572	-38.931	0.678
3100	38.573	310.749	276.881	104.991	143.196	-45.025	0.759
3200	38.617	311.974	277.958	108.850	141.818	-51.074	0.834
3300	38.660	313.163	279.007	112.714	140.438	-57.081	0.904
3400	38.703	314.318	280.029	116.582	139.059	-63.046	0.969
3500	38.746	315.440	281.025	120.455	137.680	-68.970	1.029
3600	38.789	316.532	281.996	124.332	136.304	-74.854	1.086
3700	38.831	317.596	282.944	128.213	134.931	-80.701	1.139
3800	38.873	318.632	283.869	132.098	133.564	-86.511	1.189
3900	38.915	319.642	284.774	135.987	132.203	-92.284	1.236
4000	38.957	320.628	285.658	139.881	130.850	-98.023	1.280
4100	38.999	321.590	286.522	143.779	129.505	-103.728	1.322
4200	39.040	322.531	287.369	147.681	-351.680	-102.377	1.273
4300	39.082	323.450	288.197	151.587	-351.918	-96.438	1.171
4400	39.123	324.349	289.009	155.497	-352.147	-90.494	1.074
4500	39.164	325.228	289.804	159.411	-352.365	-84.545	0.981
4600	39.205	326.090	290.583	163.330	-352.574	-78.591	0.892
4700	39.246	326.933	291.348	167.252	-352.771	-72.633	0.807
4800	39.287	327.760	292.098	171.179	-352.959	-66.670	0.726
4900	39.328	328.571	292.834	175.110	-353.135	-60.704	0.647
5000	39.369	329.365	293.557	179.045	-353.300	-54.734	0.572
5100	39.409	330.145	294.266	182.984	-353.455	-48.761	0.499
5200	39.450	330.911	294.964	186.927	-353.599	-42.786	0.430
5300	39.491	331.663	295.649	190.874	-353.732	-36.807	0.363
5400	39.531	332.401	296.323	194.825	-353.855	-30.826	0.298
5500	39.571	333.127	296.985	198.780	-353.969	-24.843	0.236
5600	39.612	333.841	297.637	202.739	-354.073	-18.858	0.176
5700	39.652	334.542	298.279	206.702	-354.168	-12.871	0.118
5800	39.693	335.232	298.910	210.669	-354.254	-6.883	0.062
5900	39.733	335.911	299.531	214.641	-354.332	-0.893	0.008
6000	39.773	336.579	300.143	218.616	-354.402	5.098	-0.044

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Bromochloroborane (BBrCl) IDEAL GAS $M_r = 126.167$ Bromochloroborane (BBrCl) $B_1Br_1Cl_1(g)$

$\Delta_f H°(0\text{ K}) = -4.3\text{ kJ·mol}^{-1}$

$S°(298.15\text{ K}) = 289.03\text{ J·K}^{-1}\text{·mol}^{-1}$ $\Delta_f H°(298.15\text{ K}) = -10.5\text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}
[660](1)
[195](1)
[905](1)

Ground State Quantum Weight: [2] $\sigma = 1$
Point Group: C_s
Bond Distances: B–Cl = [1.73] Å; B–Br = [1.87] Å
Bond Angle: Cl–B–Br = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = [2.193041\text{x } 10^{-114}]\text{ g}^3\text{·cm}^6$

Enthalpy of Formation

The enthalpy of formation is estimated by assuming $\Delta_r H° = 0$ for the reaction $BCl_2(g) + BBr_2(g) = 2\ BBrCl(g)$.

Heat Capacity and Entropy

The vibrational frequencies are estimated by comparison with those for BBr_2 and BCl_2. The bond distances, angles, and quantum weight are assumed the same as in the dihalides. The principal moments of inertia are $I_A = 1.2989 \times 10^{-39}$, $I_B = 40.4453 \times 10^{-39}$, and $I_C = 41.7442 \times 10^{-39}\text{ g·cm}^2$.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.889	−4.290	−4.290	INFINITE
100	37.800	243.541	327.661	−8.412	−3.690	−15.870	8.290
200	42.512	271.227	293.183	−4.391	−3.971	−27.994	7.311
250	44.812	280.962	289.793	−2.208	−4.376	−33.957	7.095
298.15	46.846	289.033	289.033	0.	−10.460	−38.950	6.824
300	46.919	289.323	289.034	0.087	−10.496	−39.127	6.813
350	48.726	296.695	289.612	2.479	−25.915	−43.053	6.425
400	50.221	303.303	290.917	4.954	−25.966	−45.498	5.941
450	51.439	309.291	292.631	7.497	−26.060	−47.934	5.564
500	52.429	314.763	294.575	10.094	−26.188	−50.358	5.261
600	53.895	324.461	298.769	15.415	−26.524	−55.162	4.802
700	54.891	332.848	303.052	20.858	−26.942	−59.903	4.470
800	55.589	340.226	307.247	26.384	−27.425	−64.580	4.217
900	56.093	346.804	311.283	31.969	−27.963	−69.192	4.016
1000	56.467	352.735	315.137	37.598	−28.552	−73.742	3.852
1100	56.752	358.130	318.803	43.260	−29.187	−78.231	3.715
1200	56.973	363.078	322.290	48.946	−29.866	−82.660	3.598
1300	57.147	367.646	325.605	54.653	−30.588	−87.030	3.497
1400	57.287	371.886	328.761	60.375	−31.351	−91.343	3.408
1500	57.401	375.843	331.770	66.109	−32.156	−95.601	3.329
1600	57.496	379.550	334.641	71.854	−33.001	−99.803	3.258
1700	57.574	383.038	337.387	77.608	−33.889	−103.951	3.194
1800	57.641	386.331	340.015	83.369	−34.818	−108.046	3.135
1900	57.697	389.449	342.536	89.136	−35.791	−112.088	3.082
2000	57.745	392.410	344.956	94.908	−36.808	−116.077	3.032
2100	57.787	395.228	347.283	100.684	−37.870	−120.015	2.985
2200	57.823	397.917	349.524	106.465	−38.979	−123.901	2.942
2300	57.855	400.488	351.685	112.249	−40.135	−127.735	2.901
2400	57.883	402.951	353.770	118.036	−91.600	−130.449	2.839
2500	57.907	405.315	355.785	123.825	−92.933	−132.041	2.759
2600	57.929	407.586	357.734	129.617	−94.284	−133.579	2.684
2700	57.949	409.773	359.621	135.411	−95.652	−135.064	2.613
2800	57.966	411.881	361.450	141.207	−97.040	−136.498	2.546
2900	57.982	413.915	363.224	147.004	−98.445	−137.883	2.484
3000	57.996	415.881	364.947	152.803	−99.867	−139.219	2.424
3100	58.009	417.783	366.621	158.604	−101.306	−140.507	2.368
3200	58.021	419.625	368.248	164.405	−102.761	−141.748	2.314
3300	58.032	421.410	369.832	170.208	−104.229	−142.943	2.263
3400	58.041	423.143	371.375	176.012	−105.708	−144.095	2.214
3500	58.050	424.826	372.878	181.816	−107.197	−145.202	2.167
3600	58.059	426.461	374.344	187.622	−108.694	−146.267	2.122
3700	58.066	428.052	375.774	193.428	−110.196	−147.290	2.079
3800	58.073	429.601	377.170	199.235	−111.701	−148.272	2.038
3900	58.080	431.109	378.534	205.042	−113.207	−149.215	1.999
4000	58.085	432.580	379.867	210.851	−114.711	−150.119	1.960
4100	58.091	434.014	381.170	216.659	−116.210	−150.985	1.924
4200	58.096	435.414	382.445	222.469	−597.552	−144.792	1.801
4300	58.101	436.781	383.693	228.279	−597.949	−134.007	1.628
4400	58.105	438.117	384.915	234.089	−598.337	−123.213	1.463
4500	58.110	439.423	386.112	239.900	−598.715	−112.410	1.305
4600	58.114	440.700	387.284	245.711	−599.080	−101.599	1.154
4700	58.117	441.950	388.434	251.522	−599.432	−90.781	1.009
4800	58.121	443.173	389.562	257.334	−599.768	−79.955	0.870
4900	58.124	444.372	390.668	263.147	−600.089	−69.122	0.737
5000	58.127	445.546	391.754	268.959	−600.393	−58.283	0.609
5100	58.130	446.697	392.820	274.772	−600.680	−47.438	0.486
5200	58.132	447.826	393.867	280.585	−600.948	−36.587	0.368
5300	58.135	448.933	394.896	286.398	−601.198	−25.732	0.254
5400	58.137	450.020	395.907	292.212	−601.429	−14.872	0.144
5500	58.140	451.087	396.900	298.026	−601.640	−4.007	0.038
5600	58.142	452.134	397.877	303.840	−601.833	6.860	−0.064
5700	58.144	453.163	398.838	309.654	−602.006	17.731	−0.162
5800	58.146	454.175	399.784	315.469	−602.160	28.605	−0.258
5900	58.148	455.169	400.714	321.283	−602.295	39.482	−0.350
6000	58.149	456.146	401.630	327.098	−602.412	50.360	−0.438

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Bromochloroborane (BBrCl) $B_1Br_1Cl_1(g)$

Bromodichloroborane ($BBrCl_2$) IDEAL GAS $M_r = 161.620$ Bromodichloroborane ($BBrCl_2$) $B_1Br_1Cl_2(g)$

$S°(298.15\ K) = 310.40\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -328.7 \pm 10\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = -336.8 \pm 10\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies	
υ, cm^{-1}	υ, cm^{-1}
885(1)	959 (1)
406(1)	[208](1)
218(1)	433 (1)

Ground State Quantum Weight: [1] $\sigma = 2$

Point Group: C_{2v}

Bond Distances: B–Cl = 1.73 Å; B–Br = 1.87 Å

Bond Angles: Cl–B–Cl = [120]°; Br–B–Cl = [120]°

Product of the Moments of Inertia: $I_A I_B I_C = 9.196849 \times 10^{-113}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpy of formation is estimated by assuming $\Delta_r H° = 0$ for the reaction $BBr_3(g) + 2\ BCl_3(g) = 3\ BBrCl_2(g)$.

Heat Capacity and Entropy

Vibrational frequencies are obtained from Lindeman and Wilson.[1] The b_1 mode was the only unobserved frequency and was calculated from a normal coordinate treatment. Bond distances were reported by Wentink and Tiensuu.[2] Bond angles were estimated by analogy with the other trihalides of boron. The principal moments of inertia are $I_A = 26.4297 \times 10^{-39}$, $I_B = 47.2365 \times 10^{-39}$, and $I_C = 73.6662 \times 10^{-39}\ g{\cdot}cm^{-1}$.

References

[1] L. P. Lindeman and M. K. Wilson, J. Chem. Phys. 24, 242 (1956).
[2] T. Wentink and V. H. Tiensuu, J. Chem. Phys. 28, 826 (1958).

Enthalpy Reference Temperature = T_r = 298.15 K; Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−14.547	−328.709	−328.709	INFINITE
100	42.752	252.188	361.654	−10.947	−329.442	−333.037	173.960
200	56.153	286.331	316.048	−5.943	−330.260	−336.307	87.834
250	60.770	299.375	311.440	−3.016	−330.730	−337.767	70.573
298.15	64.398	310.400	310.400	0.	−336.812	−338.417	59.289
300	64.523	310.798	310.401	0.119	−336.847	−338.427	58.925
350	67.577	320.982	311.198	3.424	−352.212	−337.848	50.421
400	70.050	330.173	313.005	6.867	−352.171	−335.799	43.851
450	72.048	338.543	315.384	10.422	−352.141	−333.754	38.741
500	73.665	346.221	318.090	14.066	−352.121	−331.712	34.654
600	76.059	359.878	323.945	21.560	−352.100	−327.633	28.523
700	77.689	371.733	329.943	29.252	−352.103	−323.555	24.144
800	78.834	382.185	335.833	37.082	−352.133	−319.475	20.860
900	79.662	391.521	341.512	45.009	−352.190	−315.390	18.305
1000	80.278	399.948	346.941	53.007	−352.277	−311.297	16.260
1100	80.747	407.622	352.114	61.059	−352.397	−307.193	14.587
1200	81.111	414.664	357.037	69.153	−352.550	−303.078	13.193
1300	81.399	421.168	361.723	77.279	−352.738	−298.947	12.012
1400	81.631	427.209	366.187	85.431	−352.962	−294.802	10.999
1500	81.819	432.848	370.446	93.604	−353.224	−290.638	10.121
1600	81.975	438.134	374.513	101.794	−353.525	−286.456	9.352
1700	82.106	443.107	378.403	109.998	−353.866	−282.254	8.673
1800	82.215	447.804	382.129	118.214	−354.249	−278.031	8.068
1900	82.309	452.251	385.704	126.440	−354.676	−273.785	7.527
2000	82.388	456.475	389.138	134.675	−355.148	−269.516	7.039
2100	82.458	460.497	392.441	142.918	−355.669	−265.222	6.597
2200	82.518	464.334	395.622	151.167	−356.240	−260.901	6.195
2300	82.570	468.003	398.690	159.421	−356.863	−256.554	5.827
2400	82.616	471.518	401.652	167.680	−407.800	−251.110	5.465
2500	82.657	474.892	404.514	175.944	−408.611	−244.564	5.110
2600	82.694	478.134	407.284	184.212	−409.447	−237.986	4.781
2700	82.726	481.256	409.966	192.483	−410.309	−231.375	4.476
2800	82.755	484.265	412.566	200.757	−411.197	−224.732	4.192
2900	82.781	487.170	415.089	209.034	−412.112	−218.056	3.928
3000	82.805	489.976	417.539	217.313	−413.053	−211.349	3.680
3100	82.826	492.692	419.919	225.595	−414.019	−204.609	3.448
3200	82.846	495.322	422.235	233.878	−415.009	−197.839	3.229
3300	82.863	497.871	424.488	242.164	−416.021	−191.036	3.024
3400	82.880	500.345	426.683	250.451	−417.053	−184.203	2.830
3500	82.894	502.748	428.822	258.739	−418.101	−177.340	2.647
3600	82.908	505.083	430.909	267.030	−419.162	−170.446	2.473
3700	82.920	507.355	432.944	275.321	−420.234	−163.522	2.309
3800	82.932	509.567	434.931	283.614	−421.313	−156.570	2.152
3900	82.943	511.721	436.873	291.907	−422.395	−149.589	2.004
4000	82.953	513.821	438.771	300.202	−423.477	−142.580	1.862
4100	82.962	515.869	440.626	308.498	−424.555	−135.544	1.727
4200	82.970	517.869	442.442	316.795	−905.475	−121.458	1.511
4300	82.978	519.821	444.218	325.092	−905.447	−102.791	1.249
4400	82.986	521.729	445.958	333.390	−905.407	−84.125	0.999
4500	82.993	523.594	447.663	341.689	−905.351	−65.460	0.760
4600	82.999	525.418	449.334	349.989	−905.277	−46.796	0.531
4700	83.005	527.203	450.971	358.289	−905.183	−28.135	0.313
4800	83.011	528.951	452.578	366.590	−905.066	−9.476	0.103
4900	83.016	530.662	454.154	374.891	−904.924	9.181	−0.098
5000	83.021	532.340	455.701	383.193	−904.755	27.835	−0.291
5100	83.026	533.984	457.220	391.495	−904.558	46.485	−0.476
5200	83.031	535.596	458.712	399.798	−904.331	65.130	−0.654
5300	83.035	537.178	460.177	408.101	−904.074	83.771	−0.826
5400	83.039	538.730	461.618	416.405	−903.785	102.407	−0.991
5500	83.043	540.253	463.034	424.709	−903.463	121.038	−1.150
5600	83.046	541.750	464.426	433.014	−903.108	139.662	−1.303
5700	83.050	543.220	465.795	441.318	−902.720	158.279	−1.450
5800	83.053	544.664	467.143	449.624	−902.299	176.890	−1.593
5900	83.056	546.084	468.469	457.929	−901.844	195.493	−1.731
6000	83.059	547.480	469.774	466.235	−901.356	214.087	−1.864

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Bromofluoroborane (BBrF) IDEAL GAS $M_r = 109.712403$

$S°(298.15\text{ K}) = [275.77]\text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0\text{ K}) = -233.9 \pm 10\text{ kJ·mol}^{-1}$

$\Delta_f H°(298.15\text{ K}) = -240.6 \pm 10\text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[860](1)
[310](1)
[1140](1)

Ground State Quantum Weight: [2] σ = 1

Point Group: C_s

Bond Distances: B–F = [1.3] Å; B–Br = [1.87] Å

Bond Angle: Br–B–F = [120]°

Product of the Moments of Inertia: $I_A I_B I_C = [4.131563 \times 10^{-115}]\text{g}^3\text{·cm}^6$

Enthalpy of Formation

The enthalpy of formation is estimated by assuming $\Delta_r H° = 0$ for the reaction $BBr_2(g) + BF_2(g) \rightarrow 2\ BBrF(g)$.

Heat Capacity and Entropy

The vibrational frequencies, bond lengths, angles and quantum weight are estimated by comparison with the respective dihalides. The principal moments of inertia are $I_A = 0.8401 \times 10^{-39}$, $I_B = 21.7603 \times 10^{-39}$, and $I_C = 22.6004 \times 10^{-39}\text{ g·cm}^2$.

Bromofluoroborane (BBrF) $B_1Br_1F_1(g)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.207	−233.906	−233.906	INFINITE
100	35.220	233.363	311.742	−7.838	−233.411	−245.506	128.239
200	39.650	259.208	279.627	−4.084	−233.905	−257.455	67.240
250	41.650	268.270	276.476	−2.051	−234.402	−263.290	55.011
298.15	43.546	275.770	275.770	0.	−240.580	−268.140	46.977
300	43.617	276.039	275.770	0.081	−240.619	−268.311	46.717
350	45.462	282.903	276.308	2.308	−256.138	−272.073	40.605
400	47.115	289.084	277.525	4.624	−256.289	−274.339	35.825
450	48.554	294.719	279.127	7.016	−256.478	−276.585	32.105
500	49.787	299.900	280.949	9.476	−256.696	−278.807	29.127
600	51.720	309.158	284.897	14.556	−257.193	−283.184	24.653
700	53.110	317.241	288.953	19.801	−257.748	−287.473	21.451
800	54.123	324.402	292.945	25.166	−258.348	−291.678	19.045
900	54.874	330.822	296.803	30.617	−258.987	−295.807	17.168
1000	55.442	336.635	300.500	36.134	−259.664	−299.862	15.663
1100	55.881	341.940	304.030	41.702	−260.378	−303.848	14.429
1200	56.225	346.818	307.395	47.307	−261.130	−307.766	13.397
1300	56.499	351.330	310.603	52.944	−261.920	−311.621	12.521
1400	56.721	355.525	313.664	58.606	−262.748	−315.413	11.768
1500	56.903	359.445	316.587	64.287	−263.616	−319.145	11.114
1600	57.054	363.122	319.381	69.985	−264.523	−322.818	10.539
1700	57.180	366.585	322.057	75.697	−265.471	−326.432	10.030
1800	57.286	369.856	324.623	81.420	−266.459	−329.990	9.576
1900	57.377	372.956	327.086	87.154	−267.487	−333.492	9.168
2000	57.456	375.901	329.453	92.895	−268.556	−336.938	8.800
2100	57.523	378.706	331.733	98.644	−269.665	−340.330	8.465
2200	57.582	381.384	333.929	104.400	−270.814	−343.668	8.160
2300	57.634	383.944	336.048	110.161	−272.001	−346.953	7.880
2400	57.679	386.398	338.096	115.926	−323.484	−349.117	7.598
2500	57.719	388.754	340.075	121.696	−324.821	−350.158	7.316
2600	57.755	391.018	341.991	127.470	−326.160	−351.145	7.055
2700	57.787	393.198	343.848	133.247	−327.499	−352.080	6.811
2800	57.816	395.300	345.648	139.027	−328.836	−352.966	6.585
2900	57.841	397.330	347.395	144.810	−330.169	−353.804	6.373
3000	57.865	399.291	349.093	150.595	−331.497	−354.597	6.174
3100	57.886	401.189	350.743	156.383	−332.818	−355.345	5.988
3200	57.905	403.027	352.348	162.173	−334.129	−356.051	5.812
3300	57.922	404.809	353.911	167.964	−335.429	−356.716	5.646
3400	57.938	406.538	355.433	173.757	−336.716	−357.341	5.490
3500	57.953	408.218	356.918	179.552	−337.989	−357.930	5.342
3600	57.967	409.851	358.365	185.348	−339.245	−358.481	5.201
3700	57.979	411.439	359.778	191.145	−340.483	−358.999	5.068
3800	57.990	412.986	361.158	196.943	−341.703	−359.483	4.941
3900	58.001	414.492	362.507	202.743	−342.902	−359.935	4.821
4000	58.011	415.961	363.825	208.543	−344.080	−360.357	4.706
4100	58.020	417.393	365.114	214.345	−345.235	−360.749	4.596
4200	58.028	418.791	366.375	220.147	−826.217	−354.090	4.404
4300	58.036	420.157	367.610	225.951	−826.238	−342.848	4.165
4400	58.044	421.491	368.820	231.755	−826.237	−331.607	3.937
4500	58.050	422.796	370.005	237.559	−826.214	−320.365	3.719
4600	58.057	424.072	371.166	243.365	−826.168	−309.125	3.510
4700	58.063	425.320	372.305	249.171	−826.099	−297.885	3.311
4800	58.069	426.543	373.423	254.977	−826.009	−286.648	3.119
4900	58.074	427.740	374.519	260.784	−825.896	−275.412	2.936
5000	58.079	428.914	375.595	266.592	−825.761	−264.179	2.760
5100	58.084	430.064	376.652	272.400	−825.606	−252.949	2.591
5200	58.088	431.192	377.690	278.209	−825.430	−241.722	2.428
5300	58.092	432.298	378.710	284.018	−825.234	−230.498	2.272
5400	58.096	433.384	379.712	289.827	−825.018	−219.279	2.121
5500	58.100	434.450	380.698	295.637	−824.784	−208.064	1.976
5600	58.104	435.497	381.667	301.447	−824.532	−196.853	1.836
5700	58.107	436.525	382.621	307.258	−824.264	−185.647	1.701
5800	58.110	437.536	383.559	313.069	−823.978	−174.446	1.571
5900	58.113	438.529	384.482	318.880	−823.678	−163.249	1.445
6000	58.116	439.506	385.391	324.691	−823.363	−152.058	1.324

PREVIOUS· December 1964 (1 atm)   CURRENT: December 1964 (1 bar)

Bromofluoroborane (BBrF) $B_1Br_1F_1(g)$

Bromodifluoroborane ($BBrF_2$) IDEAL GAS $M_r = 128.710806$ Bromodifluoroborane ($BBrF_2$) $B_1Br_1F_2(g)$

$S°(298.15 K) = 286.39 J·K^{-1}·mol^{-1}$

$\Delta_f H°(0 K) = [-811 \pm 10] kJ·mol^{-1}$
$\Delta_f H°(298.15 K) = [-820 \pm 10] kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}
1215 (1)	1427 (1)
633 (1)	[346](1)
[330](1)	573 (1)

Ground State Quantum Weight: [1] $\sigma = 2$
Point Group: C_{2v}
Bond Distances: B–F = 1.295 Å; B–Br = 1.87 Å
Bond Angles: F–B–F = [120]°; Br–B–F = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = 8.471599 \times 10^{-114}$ g^3·cm^6

Enthalpy of Formation

The enthalpy of formation is estimated by assuming $\Delta_r H° = 0$ for the reaction $2 BF_3(g) + BBr_3(g) \rightarrow 3 BBrF_2(g)$.

Heat Capacity and Entropy

All but two of the vibrational frequencies have been observed and assigned by Lindeman and Wilson.[1] The two remaining frequencies were calculated by a normal coordinate treatment. The bond distances were reported by Wentink and Tiensuu.[2] The bond angles were estimated by analogy with the other boron trihalides. The principal moments of inertia are $I_A = 7.9360 \times 10^{-39}$, $I_B = 28.9444 \times 10^{-39}$, and $I_C = 36.8805 \times 10^{-39}$ g·cm^2.

References

[1] L. P. Lindeman and M. K. Wilson, J. Chem. Phys. 24, 242 (1956).
[2] T. Wentink and V. H. Tiensuu, J. Chem. Phys. 28, 826 (1958).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	−12.778	−810.549	−810.549	INFINITE
100	36.575	236.647	330.512	−9.387	−811.485	−815.389	425.916
200	47.998	265.547	291.299	−5.150	−812.961	−818.714	213.826
250	52.679	276.777	287.296	−2.630	−813.722	−820.066	171.343
298.15	56.450	286.387	286.387	0.	−820.064	−820.559	143.759
300	56.583	286.737	286.388	0.105	−820.108	−820.562	142.873
350	59.897	295.715	287.090	3.019	−835.735	−819.775	122.345
400	62.745	303.903	288.687	6.087	−835.948	−817.480	106.752
450	65.198	311.439	290.802	9.287	−836.164	−815.159	94.621
500	67.311	318.420	293.219	12.601	−836.376	−812.813	84.914
600	70.693	331.007	298.491	19.509	−836.782	−808.062	70.348
700	73.200	342.102	303.945	26.710	−837.157	−803.245	59.939
800	75.075	352.005	309.344	34.128	−837.508	−798.376	52.129
900	76.495	360.933	314.589	41.710	−837.844	−793.465	46.051
1000	77.589	369.052	319.635	49.417	−838.177	−788.516	41.188
1100	78.444	376.489	324.470	57.220	−838.515	−783.534	37.207
1200	79.122	383.344	329.095	65.099	−838.866	−778.520	33.888
1300	79.667	389.700	333.515	73.040	−839.237	−773.476	31.079
1400	80.111	395.620	337.742	81.029	−839.632	−768.403	28.669
1500	80.477	401.160	341.787	89.059	−840.056	−763.301	26.580
1600	80.781	406.364	345.662	97.123	−840.513	−758.169	24.752
1700	81.038	411.269	349.379	105.214	−841.003	−753.007	23.137
1800	81.255	415.908	352.947	113.329	−841.530	−747.816	21.701
1900	81.440	420.306	356.378	121.464	−842.093	−742.595	20.415
2000	81.600	424.488	359.679	129.616	−842.692	−737.343	19.257
2100	81.739	428.472	362.861	137.783	−843.326	−732.060	18.209
2200	81.860	432.278	365.931	145.963	−843.995	−726.746	17.255
2300	81.966	435.919	368.895	154.155	−844.695	−721.401	16.384
2400	82.060	439.409	371.761	162.356	−895.684	−714.956	15.561
2500	82.143	442.761	374.534	170.566	−896.519	−707.408	14.780
2600	82.217	445.984	377.221	178.785	−897.344	−699.827	14.060
2700	82.283	449.088	379.825	187.010	−898.159	−692.215	13.392
2800	82.342	452.082	382.353	195.241	−898.958	−684.573	12.771
2900	82.395	454.972	384.807	203.478	−899.740	−676.902	12.192
3000	82.444	457.766	387.193	211.720	−900.502	−669.205	11.652
3100	82.487	460.470	389.513	219.966	−901.241	−661.483	11.146
3200	82.527	463.090	391.772	228.217	−901.954	−653.738	10.671
3300	82.564	465.630	393.972	236.472	−902.639	−645.970	10.225
3400	82.597	468.095	396.116	244.730	−903.293	−638.183	9.804
3500	82.627	470.490	398.207	252.991	−903.915	−630.376	9.408
3600	82.655	472.818	400.247	261.255	−904.502	−622.552	9.033
3700	82.681	475.083	402.239	269.522	−905.053	−614.712	8.678
3800	82.705	477.288	404.185	277.791	−905.567	−606.859	8.342
3900	82.727	479.437	406.087	286.063	−906.043	−598.991	8.023
4000	82.747	481.532	407.947	294.336	−906.478	−591.113	7.719
4100	82.766	483.575	409 767	302.612	−906.874	−583.224	7.430
4200	82.784	485.570	411.548	310.890	−1387.078	−568.301	7.068
4300	82.800	487.518	413.293	319.169	−1386.304	−548.816	6.667
4400	82.816	489.422	415.001	327.450	−1385.491	−529.349	6.284
4500	82.830	491.283	416.676	335.732	−1384.638	−509.900	5.919
4600	82.843	493.104	418.318	344.016	−1383.746	−490.471	5.569
4700	82.856	494.885	419.928	352.301	−1382.816	−471.062	5.235
4800	82.868	496.630	421.508	360.587	−1381.847	−451.673	4.915
4900	82.879	498.339	423.058	368.874	−1380.842	−432.305	4.608
5000	82.889	500.013	424.581	377.162	−1379.800	−412.958	4.314
5100	82.899	501.655	426.076	385.452	−1378.722	−393.631	4.032
5200	82.908	503.264	427.545	393.742	−1377.610	−374.327	3.760
5300	82.917	504.844	428.988	402.034	−1376.464	−355.044	3.499
5400	82.925	506.394	430.408	410.326	−1375.285	−335.783	3.248
5500	82.933	507.915	431.803	418.619	−1374.075	−316.544	3.006
5600	82.941	509.410	433.175	426.912	−1372.835	−297.327	2.773
5700	82.948	510.878	434.526	435.207	−1371.566	−278.133	2.549
5800	82.954	512.321	435.855	443.502	−1370.269	−258.961	2.332
5900	82.961	513.739	437.163	451.798	−1368.945	−239.812	2.123
6000	82.967	515.133	438.451	460.094	−1367.596	−220.686	1.921

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

M_r = 106.7134

$S°(298.15\ K) = [248.89]\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = [-244 \pm 7]\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [-251 \pm 7]\ kJ\cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[550](1)
[370](2)
[1800](1)

Ground State Quantum Weight: [1]
Point Group: [$C_{\infty v}$]
Bond Distances: O–B = [1.20] Å; B–Br = [1.87] Å
Bond Angle: O–B–Br = [180]°
Rotation Constant: B_0 = [0.117436] cm^{-1}
$\alpha = 1$

Enthalpy of Formation

The value of $\Delta_f H°$(BOBr, g, 298.15 K) is calculated based on an assumption that $D_0°$(BO–Br) = 92.5 kcal·mol^{-1} which is estimated by comparison with the following related bond energy values: $D_0°$(BF$_2$–F) = 159, $D_0°$(BO–F) = 169, $D_0°$(BCl$_2$–Cl) = 105, $D_0°$(BO–Cl) = 110 and $D_0°$(BBr$_2$–Br) = 90.5 kcal·mol^{-1}.

Heat Capacity and Entropy

The molecular structure is assumed to be linear. The vibrational frequencies (ν) are estimated from the ν values calculated by the valence force method by Herzberg[1] using estimated force constants, $k_1 = 4.2 \times 105$, $k_2 = 16.9 \times 105$ dynes cm^{-1} and $k_g = 0.37 \times 10^{-11}$ dynes·cm·rad^{-1}. The B=O and B–F[1] bond distances are assumed to be the same as those in BO(g) and BBr$_3$(g), respectively.

Reference

[1] G. Herzberg, Infrared and Raman Spectra, D. Van Nostrand Company, Inc., (1945).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	S°	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.961	−244.191	−244.191	INFINITE
100	31.611	206.321	286.380	−8.006	−244.108	−253.352	132.338
200	41.199	231.278	253.022	−4.349	−244.690	−262.372	68.524
250	44.510	240.848	249.654	−2.201	−245.051	−266.753	55.735
298.15	46.810	248.895	248.895	0.	−251.040	−270.236	47.344
300	46.885	249.185	248.896	0.087	−251.072	−270.355	47.073
350	48.664	256.552	249.474	2.477	−266.371	−272.732	40.703
400	50.078	263.145	250.778	4.947	−266.299	−273.647	35.735
450	51.262	269.114	252.489	7.481	−266.272	−274.567	31.871
500	52.290	274.569	254.428	10.071	−266.282	−275.489	28.780
600	54.011	284.261	258.612	15.389	−266.384	−277.322	24.143
700	55.392	292.694	262.892	20.862	−266.563	−279.132	20.829
800	56.505	300.166	267.093	26.459	−266.794	−280.912	18.342
900	57.401	306.875	271.147	32.155	−267.063	−282.661	16.405
1000	58.127	312.962	275.029	37.933	−267.366	−284.378	14.854
1100	58.716	318.530	278.734	43.776	−267.699	−286.063	13.584
1200	59.198	323.661	282.267	49.673	−268.062	−287.717	12.524
1300	59.596	328.415	285.636	55.613	−268.455	−289.339	11.626
1400	59.927	332.844	288.852	61.590	−268.879	−290.930	10.855
1500	60.204	336.989	291.924	67.597	−269.337	−292.489	10.185
1600	60.438	340.882	294.864	73.629	−269.829	−294.017	9.599
1700	60.637	344.552	297.680	79.683	−270.357	−295.513	9.080
1800	60.808	348.023	300.381	85.756	−270.924	−296.976	8.618
1900	60.955	351.314	302.976	91.844	−271.532	−298.407	8.204
2000	61.082	354.444	305.471	97.946	−272.181	−299.805	7.830
2100	61.193	357.427	307.875	104.060	−272.875	−301.169	7.491
2200	61.291	360.276	310.193	110.184	−273.613	−302.499	7.182
2300	61.377	363.003	312.430	116.317	−274.399	−303.795	6.899
2400	61.453	365.617	314.592	122.459	−325.491	−303.987	6.616
2500	61.521	368.127	316 684	128.608	−326.450	−303.071	6.332
2600	61.582	370.541	318.709	134.763	−327.424	−302.117	6.070
2700	61.636	372.866	320.672	140.924	−328.415	−301.125	5.826
2800	61.685	375.108	322.576	147.090	−329.421	−300.096	5.598
2900	61.729	377.274	324.425	153.261	−330.442	−299.031	5.386
3000	61.769	379.367	326.222	159.436	−331.479	−297.930	5.187
3100	61.805	381.393	327.969	165.614	−332.529	−296.794	5.001
3200	61.838	383.356	329.669	171.797	−333.591	−295.624	4.826
3300	61.868	385.259	331.325	177.982	−334.665	−294.422	4.660
3400	61.896	387.107	332.939	184.170	−335.748	−293.186	4.504
3500	61.922	388.901	334.512	190.361	−336.841	−291.918	4.357
3600	61.945	390.646	336.047	196.554	−337.940	−290.619	4.217
3700	61.966	392.343	337.546	202.750	−339.045	−289.289	4.084
3800	61.986	393.996	339.010	208.948	−340.154	−287.929	3.958
3900	62.005	395.607	340.441	215.147	−341.266	−286.541	3.838
4000	62.022	397.177	341.839	221.349	−342.379	−285.123	3.723
4100	62.038	398.708	343.208	227.552	−343.493	−283.678	3.614
4200	62.053	400.203	344.547	233.756	−824.456	−275.182	3.422
4300	62.067	401.664	345.859	239.962	−824.481	−262.103	3.184
4400	62.079	403.091	347.143	246.169	−824.506	−249.025	2.956
4500	62.092	404.486	348.402	252.378	−824.529	−235.945	2.739
4600	62.103	405.851	349.636	258.588	−824.551	−222.866	2.531
4700	62.113	407.187	350.846	264.799	−824.572	−209.785	2.332
4800	62.123	408.494	352.034	271.010	−824.591	−196.704	2.141
4900	62.133	409.775	353.199	277.223	−824.609	−183.623	1.957
5000	62.142	411.031	354.343	283.437	−824.626	−170.541	1.782
5100	62.150	412.261	355.467	289.652	−824.642	−157.459	1.613
5200	62.158	413.468	356.571	295.867	−824.658	−144.378	1.450
5300	62.165	414.652	357.656	302.083	−824.674	−131.295	1.294
5400	62.172	415.814	358.722	308.300	−824.691	−118.212	1.143
5500	62.179	416.955	359.770	314.517	−824.709	−105.129	0.998
5600	62.185	418.076	360.802	320.736	−824.729	−92.046	0.859
5700	62.191	419.176	361.816	326.955	−824.753	−78.962	0.724
5800	62.197	420.258	362.814	333.174	−824.781	−65.877	0.593
5900	62.202	421.321	363.797	339.394	−824.814	−52.793	0.467
6000	62.207	422.367	364.764	345.614	−824.853	−39.707	0.346

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

Dibromoborane (BBr_2) IDEAL GAS M_r = 170.618 Dibromoborane (BBr_2) $B_1Br_2(g)$

$S°(298.15\ K) = [294.66]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [76.3 \pm 15]\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = [62.8 \pm 15]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[600](1)
[150](1)
[830](1)

Ground State Quantum Weight: [2] $\sigma = 2$
Point Group: [C_{2v}]
Bond Distance: B–Br = [1.87] Å
Bond Angle: Br–B–Br = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = [7.270321 \times 10^{-114}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpy of formation is estimated by analogy with BF_3, specifically the ratio $\Delta_rH°(BX_3 \rightarrow BX_2 + X)/\Delta_rH°(BX_3 \rightarrow B + 3X)$ is taken as 0.347.

Heat Capacity and Entropy

The vibrational frequencies were obtained from force constants transferred from the trihalide given by Herzberg.[1] The bond length is taken between those of the mono and trihalide and the angle is estimated to be the same as that in the trihalides. The ground state quantum weight is taken as two due to the one unpaired electron.

The principal moments of inertia are $I_A = 1.4699 \times 10^{-39}$, $I_B = 69.5984 \times 10^{-39}$, and $I_C = 71.0683 \times 10^{-39}\ g{\cdot}cm^2$.

Reference

[1] G. Herzberg, Infrared and Raman Spectra of Polyatomic Molecules, D. Van Nostrand Inc., (1945).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−12.209	76.274	76.274	INFINITE
100	39.095	247.877	334.353	−8.648	77.019	57.646	−30.111
200	43.694	276.369	298.924	−4.511	75.921	38.615	−10.085
250	46.046	286.375	295.442	−2.267	74.979	29.392	−6.141
298.15	48.056	294.662	294.662	0.	62.760	22.026	−3.859
300	48.127	294.959	294.663	0.089	62.688	21.774	−3.791
350	49.854	302.512	295.255	2.540	31.862	16.646	−2.484
400	51.245	309.264	296.592	5.069	31.825	14.475	−1.890
450	52.357	315.366	298.344	7.660	31.747	12.310	−1.429
500	53.245	320.930	300.329	10.301	31.635	10.156	−1.061
600	54.539	330.760	304.603	15.694	31.328	5.888	−0.513
700	55.403	339.237	308.959	21.194	30.934	1.678	−0.125
800	56.003	346.676	313.218	26.766	30.471	−2.471	0.161
900	56.432	353.299	317.311	32.389	29.948	−6.557	0.381
1000	56.750	359.262	321.213	38.049	29.371	−10.583	0.553
1100	56.990	364.682	324.922	43.737	28.746	−14.549	0.691
1200	57.176	369.649	328.445	49.445	28.074	−18.455	0.803
1300	57.322	374.232	331.793	55.170	27.357	−22.304	0.896
1400	57.440	378.484	334.978	60.909	26.596	−26.096	0.974
1500	57.535	382.451	338.012	66.658	25.792	−29.832	1.039
1600	57.614	386.166	340.907	72.415	24.944	−33.512	1.094
1700	57.680	389.661	343.673	78.180	24.051	−37.139	1.141
1800	57.735	392.960	346.320	83.951	23.114	−40.711	1.181
1900	57.782	396.083	348.858	89.727	22.129	−44.230	1.216
2000	57.822	399.047	351.294	95.507	21.096	−47.697	1.246
2100	57.857	401.869	353.636	101.291	20.014	−51.110	1.271
2200	57.887	404.562	355.890	107.078	18.880	−54.470	1.293
2300	57.914	407.135	358.062	112.868	17.694	−57.778	1.312
2400	57.937	409.601	360.159	118.661	−33.805	−59.964	1.305
2500	57.957	411.966	362.184	124.455	−35.175	−61.026	1.275
2600	57.975	414.240	364.143	130.252	−36.567	−62.033	1.246
2700	57.992	416.428	366.039	136.050	−37.979	−62.985	1.219
2800	58.006	418.537	367.877	141.850	−39.411	−63.886	1.192
2900	58.019	420.573	369.659	147.652	−40.861	−64.734	1.166
3000	58.031	422.540	371.389	153.454	−42.329	−65.532	1.141
3100	58.042	424.443	373.070	159.258	−43.812	−66.281	1.117
3200	58.052	426.286	374.704	165.063	−45.308	−66.982	1.093
3300	58.061	428.073	376.294	170.868	−46.814	−67.636	1.071
3400	58.069	429.806	377.843	176.675	−48.329	−68.245	1.048
3500	58.076	431.489	379.352	182.482	−49.849	−68.808	1.027
3600	58.083	433.126	380.823	188.290	−51.372	−69.328	1.006
3700	58.089	434.717	382.258	194.098	−52.895	−69.806	0.985
3800	58.095	436.266	383.659	199.908	−54.416	−70.243	0.966
3900	58.100	437.775	385.027	205.717	−55.932	−70.640	0.946
4000	58.105	439.246	386.365	211.528	−57.441	−70.998	0.927
4100	58.110	440.681	387.672	217.338	−58.941	−71.318	0.909
4200	58.114	442.082	388.951	223.150	−540.279	−64.578	0.803
4300	58.118	443.449	390.202	228.961	−540.668	−53.247	0.647
4400	58.122	444.785	391.428	234.773	−541.044	−41.907	0.498
4500	58.125	446.091	392.628	240.586	−541.406	−30.559	0.355
4600	58.128	447.369	393.804	246.398	−541.753	−19.203	0.218
4700	58.131	448.619	394.957	252.211	−542.084	−7.840	0.087
4800	58.134	449.843	396.088	258.025	−542.399	3.531	−0.038
4900	58.137	451.042	397.197	263.838	−542.696	14.907	−0.159
5000	58.140	452.216	398.286	269.652	−542.977	26.290	−0.275
5100	58.142	453.368	399.355	275.466	−543.240	37.678	−0.386
5200	58.144	454.497	400.404	281.280	−543.486	49.071	−0.493
5300	58.146	455.604	401.435	287.095	−543.714	60.469	−0.596
5400	58.148	456.691	402.449	292.910	−543.925	71.870	−0.695
5500	58.150	457.758	403.445	298.724	−544.119	83.276	−0.791
5600	58.152	458.806	404.424	304.540	−544.296	94.684	−0.883
5700	58.154	459.835	405.387	310.355	−544.458	106.096	−0.972
5800	58.155	460.847	406.335	316.170	−544.603	117.510	−1.058
5900	58.157	461.841	407.267	321.986	−544.734	128.927	−1.141
6000	58.158	462.818	408.185	327.802	−544.850	140.346	−1.222

PREVIOUS: December 1964 (1 atm) CURRENT· December 1964 (1 bar)

Dibromochloroborane (BBr_2Cl) IDEAL GAS $M_r = 206.071$

$S°(298.15\ K) = 321.89\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = [-257 \pm 10]\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [-272 \pm 10]\ kJ\cdot mol^{-1}$

Vibrational Levels and Degeneracies υ, cm^{-1}	 υ, cm^{-1}
925(1)	834(1)
344(1)	195(1)
166(1)	409(1)

Ground State Quantum Weight: [1] $\sigma = 2$
Point Group: C_{2v}
Bond Distances: B–Br = 1.87 Å; B–Cl = 1.75 Å
Bond Angles: Br–B–Br = [120]°; Cl–B–Br = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = 2.555411 \times 10^{-112}\ g^3\cdot cm^6$

Enthalpy of Formation

The enthalpy of formation is estimated by assuming $\Delta_r H° = 0$ for the reaction $2\ BBr_3(g) + BCl_3(g) \rightarrow 3\ BBr_2Cl(g)$.

Heat Capacity and Entropy

The vibrational frequencies have all been observed and assigned by Lindeman and Wilson.[1] The bond lengths were reported by Wentink and Tiensuu.[2] Bond angles are estimated by analogy with the other trihalides of boron. The principal moments of inertia are $I_A = 35.0767 \times 10^{-39}$, $I_B = 69.5984 \times 10^{-39}$, and $I_C = 104.6751 \times 10^{-39}\ g\cdot cm^2$.

References

[1] L. P. Lindeman and M. K. Wilson, J. Chem. Phys. 24, 242 (1956).
[2] T. Wentink and V. H. Tiensuu, J. Chem. Phys. 28, 826 (1958).

Dibromochloroborane (BBr_2Cl) $B_1Br_2Cl_1(g)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−15.092	−256.738	−256.738	INFINITE
100	45.297	261.227	374.950	−11.372	−257.292	−268.549	140.275
200	58.289	297.067	327.702	−6.127	−258.799	−279.248	72.932
250	62.626	310.557	322.958	−3.100	−259.769	−284.253	59.391
298.15	66.028	321.889	321.889	0.	−271.960	−287.556	50.379
300	66.145	322.298	321.890	0.122	−272.030	−287.652	50.085
350	68.994	332.716	322.707	3.503	−302.786	−288.570	43.067
400	71.286	342.084	324.553	7.012	−302.717	−286.544	37.419
450	73.127	350.591	326.981	10.624	−302.663	−284.525	33.027
500	74.609	358.375	329.736	14.319	−302.619	−282.512	29.514
600	76.790	372.184	335.690	21.896	−302.558	−278.497	24.245
700	78.265	384.139	341.776	29.654	−302.531	−274.490	20.483
800	79.296	394.661	347.742	37.535	−302.535	−270.484	17.661
900	80.040	404.046	353.486	45.503	−302.572	−266.476	15.466
1000	80.591	412.509	358.972	53.536	−302.644	−262.462	13.710
1100	81.010	420.211	364.195	61.617	−302.751	−258.439	12.272
1200	81.336	427.274	369.161	69.735	−302.895	−254.404	11.074
1300	81.593	433.795	373.885	77.882	−303.076	−250.356	10.059
1400	81.799	439.849	378.383	86.052	−303.296	−246.293	9.189
1500	81.967	445.499	382.672	94.241	−303.556	−242.212	8.435
1600	82.106	450.793	386.765	102.445	−303.858	−238.113	7.774
1700	82.222	455.775	390.680	110.661	−304.202	−233.994	7.190
1800	82.319	460.477	394.428	118.888	−304.593	−229.853	6.670
1900	82.402	464.930	398.022	127.125	−305.030	−225.689	6.205
2000	82.473	469.159	401.474	135.369	−305.518	−221.501	5.785
2100	82.535	473.184	404.794	143.619	−306.059	−217.287	5.405
2200	82.588	477.025	407.991	151.875	−306.654	−213.046	5.058
2300	82.635	480.697	411.073	160.136	−307.306	−208.777	4.741
2400	82.676	484.215	414.047	168.402	−358.275	−203.409	4.427
2500	82.712	487.591	416.922	176.671	−359.124	−196.939	4.115
2600	82.745	490.835	419.703	184.944	−360.000	−190.434	3.826
2700	82.773	493.959	422.396	193.220	−360.904	−183.895	3.558
2800	82.799	496.969	425.006	201.499	−361.837	−177.322	3.308
2900	82.822	499.875	427.537	209.780	−362.797	−170.716	3.075
3000	82.843	502.684	429.996	218.063	−363.783	−164.076	2.857
3100	82.862	505.400	432.385	226.349	−364.793	−157.402	2.652
3200	82.879	508.031	434.708	234.636	−365.824	−150.696	2.460
3300	82.895	510.582	436.968	242.924	−366.875	−143.956	2.279
3400	82.909	513.057	439.170	251.215	−367.941	−137.186	2.108
3500	82.923	515.460	441.316	259.506	−369.019	−130.383	1.946
3600	82.935	517.797	443.408	267.799	−370.107	−123.549	1.793
3700	82.946	520.069	445.449	276.093	−371.199	−116.685	1.647
3800	82.956	522.281	447.442	284.388	−372.294	−109.792	1.509
3900	82.966	524.436	449.389	292.684	−373.386	−102.870	1.378
4000	82.974	526.537	451.291	300.981	−374.473	−95.920	1.253
4100	82.982	528.586	453.152	309.279	−375.552	−88.943	1.133
4200	82.990	530.585	454.972	317.578	−856.467	−74.915	0.932
4300	82.997	532.538	456.753	325.877	−856.431	−56.307	0.684
4400	83.004	534.446	458.497	334.177	−856.378	−37.700	0.448
4500	83.010	536.312	460.206	342.478	−856.307	−19.095	0.222
4600	83.016	538.136	461.880	350.779	−856.215	−0.491	0.006
4700	83.021	539.922	463.522	359.081	−856.100	18.111	−0.201
4800	83.026	541.670	465.132	367.383	−855.961	36.710	−0.399
4900	83.031	543.382	466.711	375.686	−855.796	55.305	−0.590
5000	83.035	545.059	468.261	383.989	−855.603	73.897	−0.772
5100	83.039	546.704	469.783	392.293	−855.382	92.485	−0.947
5200	83.043	548.316	471.278	400.597	−855.133	111.068	−1.116
5300	83.047	549.898	472.747	408.902	−854.854	129.647	−1.278
5400	83.051	551.450	474.190	417.207	−854.544	148.219	−1.434
5500	83.054	552.974	475.608	425.512	−854.205	166.786	−1.584
5600	83.057	554.471	477.003	433.818	−853.835	185.346	−1.729
5700	83.060	555.941	478.375	442.123	−853.436	203.899	−1.869
5800	83.063	557.385	479.725	450.430	−853.006	222.445	−2.003
5900	83.066	558.805	481.054	458.736	−852.546	240.983	−2.134
6000	83.068	560.202	482.361	467.043	−852.058	259.514	−2.259

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Dibromochloroborane (BBr_2Cl) $B_1Br_2Cl_1(g)$

Dibromofluoroborane (BBr_2F) IDEAL GAS M_r = 189.616403 Dibromofluoroborane (BBr_2F) $B_1Br_2F_1(g)$

$S°(298.15 K) = [309.99] J·K^{-1}·mol^{-1}$

$\Delta_fH°(0 K) = [-499 \pm 10] kJ·mol^{-1}$
$\Delta_fH°(298.15 K) = [-515 \pm 10] kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}	υ, cm^{-1}
1310(1)	869 (1)
[418](1)	[283](1)
[183](1)	[496](1)

Ground State Quantum Weight: [1] σ = 2
Point Group: C_{2v}
Bond Distances: B–Br = 1.87 Å; B–Cl = 1.295 Å
Bond Angles: Br–B–Br = [120]°; Br–B–F = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = 8.725604 \times 10^{-113} g^3·cm^6$

Enthalpy of Formation

The enthalpy of formation is estimated by assuming $\Delta_rH° = 0$ for the reaction 2 $BBr_3(g) + BF_3(g) \rightarrow 3 BBr_2F(g)$.

Heat Capacity and Entropy

Two of the vibrational frequencies were observed and assigned by Lindeman and Wilson.[1] The remaining frequencies were calculated by a normal coordinate treatment using force constants obtained by comparison with the other mixed trihalides. The bond distances were reported by Wentink and Tiensuu.[2] The bond angles are estimated by analogy with the other trihalides. The principal moments of inertia are $I_A = 14.8465 \times 10^{-39}$, $I_B = 69.5984 \times 10^{-39}$, and $I_C = 84.4449 \times 10^{-39} g·cm^2$.

References

[1] L. P. Lindeman and M. K. Wilson, J. Chem. Phys. 24, 242 (1956).
[2] T. Wentink and V. H. Tiensuu, J. Chem. Phys. 28, 826 (1958).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	S°	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−14.170	−498.666	−498.666	INFINITE
100	41.579	253.624	359.617	−10.599	−499.366	−510.795	266.812
200	54.385	286.688	315.462	−5.755	−501.220	−521.525	136.208
250	58.848	299.322	311.001	−2.920	−502.323	−526.478	110.001
298.15	62.316	309.994	309.994	0.	−514.632	−529.706	92.802
300	62.436	310.380	309.995	0.115	−514.707	−529.799	92.246
350	65.384	320.233	310.766	3.313	−545.581	−530 619	79.191
400	67.832	329.128	312.515	6.645	−545.629	−528.478	69.012
450	69.875	337.239	314.818	10.090	−545.687	−526.331	61.095
500	71.585	344.692	317.438	13.627	−545.752	−524 177	54.760
600	74.230	357.991	323.115	20.926	−545.891	−519.849	45.257
700	76.122	369.584	328.943	28.448	−546.038	−515 497	38.467
800	77.502	379.843	334.677	36.133	−546.193	−511.124	33.373
900	78.530	389 034	340.215	43.937	−546.362	−506.730	29.410
1000	79.310	397.350	345.519	51.831	−546.550	−502.317	26.238
1100	79.913	404.939	350.581	59.793	−546.760	−497.884	23.643
1200	80.388	411.913	355.406	67.809	−546.998	−493.430	21.478
1300	80.768	418.363	360.003	75.868	−547.266	−488.955	19.646
1400	81.076	424.360	364.389	83.960	−547.568	−484.459	18.075
1500	81.329	429.963	368.576	92.081	−547.906	−479.939	16.713
1600	81.538	435.219	372.578	100.225	−548.282	−475.396	15.520
1700	81.714	440.167	376.410	108.388	−548.699	−470.828	14.467
1800	81.863	444.842	380.083	116.567	−549.158	−466.235	13.530
1900	81.990	449.272	383.609	124.759	−549.662	−461.614	12.691
2000	82.099	453.480	386.998	132.964	−550.211	−456.966	11.935
2100	82.193	457.488	390.260	141.179	−550.806	−452.289	11.250
2200	82.276	461.314	393.404	149.402	−551.448	−447.583	10.627
2300	82.348	464.973	396.436	157.633	−552.137	−442.847	10.057
2400	82.411	468.479	399.366	165.872	−603.132	−437.010	9.511
2500	82.468	471.844	402.198	174.116	−603.991	−430.071	8.986
2600	82.518	475.080	404.939	182.365	−604.861	−423.097	8.500
2700	82.563	478.195	407.595	190.619	−605.740	−416.090	8.050
2800	82.603	481.198	410.171	198.877	−606.628	−409.050	7.631
2900	82.639	484.097	412.670	207.139	−607.520	−401.977	7.240
3000	82.672	486.900	415.098	215.405	−608.416	−394 874	6.875
3100	82.701	489.611	417.458	223.674	−609.311	−387.742	6.533
3200	82.728	492.237	419.754	231.945	−610.203	−380.580	6.212
3300	82.753	494.783	421.989	240.219	−611.089	−373.391	5.910
3400	82.775	497.254	424.167	248.496	−611.966	−366.174	5.626
3500	82.796	499.653	426.289	256.774	−612.830	−358.933	5.357
3600	82.815	501.986	428.360	265.055	−613.680	−351.666	5.103
3700	82.832	504.255	430.381	273.337	−614.512	−344.377	4.862
3800	82.848	506.465	432.354	281.621	−615.323	−337.065	4.633
3900	82.863	508.617	434.282	289.907	−616.111	−329.732	4.416
4000	82.877	510.715	436.167	298.194	−616.875	−322.379	4.210
4100	82.890	512.762	438.010	306.482	−617.611	−315.008	4.013
4200	82.901	514.759	439.814	314.771	−1098.169	−300.594	3.738
4300	82.913	516.710	441.579	323.062	−1097.759	−281.609	3.421
4400	82.923	518.616	443.308	331.354	−1097.319	−262.634	3.118
4500	82.933	520.480	445.003	339.647	−1096.849	−243.669	2.828
4600	82.942	522.303	446.663	347.940	−1096.348	−224.715	2.552
4700	82.950	524.087	448.292	356.235	−1095.814	−205.772	2.287
4800	82.958	525.833	449.889	364.530	−1095.249	−186.841	2.033
4900	82.965	527.544	451.457	372.827	−1094.652	−167.922	1.790
5000	82.973	529.220	452.995	381.123	−1094.022	−149.015	1.557
5100	82.979	530.863	454.506	389.421	−1093.361	−130.122	1.333
5200	82.985	532.474	455.990	397.719	−1092.668	−111.241	1.117
5300	82.991	534.055	457.448	406.018	−1091.944	−92.374	0.910
5400	82.997	535.606	458.881	414.318	−1091.190	−73.522	0.711
5500	83.002	537.129	460.290	422.618	−1090.407	−54.683	0.519
5600	83.007	538.625	461.675	430.918	−1089.594	−35.859	0.334
5700	83.012	540.094	463.038	439.219	−1088.753	−17.050	0.156
5800	83.016	541.538	464.379	447.520	−1087.885	1.744	−0.016
5900	83.021	542.957	465.699	455.822	−1086.991	20.523	−0.182
6000	83.025	544.353	466.998	464.124	−1086.071	39.287	−0.342

PREVIOUS: December 1964 (1 atm) CURRENT. December 1964 (1 bar)

Dibromoborane ($BHBr_2$) IDEAL GAS $M_r = 171.62594$ Dibromoborane ($BHBr_2$) $B_1Br_2H_1(g)$

$\Delta_f H°(0\ K) = [-87 \pm 5]\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = [292.27]\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = [-105 \pm 5]\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}	υ, cm^{-1}
2600 (1)	1044(1)
[532](1)	775(1)
[158](1)	783(1)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: B–H = 1.20 Å; B–Br = [1.87] Å
Bond Angles: Br–B–Br = 119.3 ± 2°; Br–B–H = 120.3 ± 1°
Product of the Moments of Inertia: $I_A I_B I_C = 1.096494 \times 10^{-113}\ g^3 \cdot cm^6$

Enthalpy of Formation

The value of $\Delta_f H°(BBr_2H, g, 298.15\ K)$ is derived by assuming the B–H bond strength to be 92 kcal·mol^{-1}, the same as that in $BCl_2H(g)$.

Heat Capacity and Entropy

The molecular structure, B–H bond distance and bond angle were obtained from Lynds and Bass.[1] The B–Br bond distance is taken from that in $BBr_3(g)$ molecule. The vibrational frequencies adopted and corrected to the average isotopic species were assigned to Brieux de Mandirola and Westerkamp[2] from infrared spectrum. The values in brackets are calculated by the Wilson's FG method. Infrared spectrum of $BBr_2H(g)$ was also reported by Wason and Porter[3] and three frequencies, υ_1, υ_4, and υ_5, were assigned. The principal moments of inertia are: $I_A = 2.2244 \times 10^{-39}$, $I_B = 69.1057 \times 10^{-39}$, and $I_C = 71.3302 \times 10^{-39}\ g \cdot cm^2$.

References

[1] L. Lynds and C. D. Bass, J. Phys. Chem. **41**, 3165 (1964).
[2] O. Brieux de Mandirola and J. F. Westerkamp, Spectrochim. Acta **21**, 1101 (1965).
[3] S. K. Wason and R. F. Porter, J. Phys. Chem. **69**, 2461 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−12.624	−87.267	−87.267	INFINITE
100	39.016	243.626	334.406	−9.078	−88.038	−101.949	53.252
200	45.697	272.588	296.897	−4.862	−90.403	−115.011	30.038
250	49.642	283.208	293.122	−2.478	−91.904	−120.994	25.280
298.15	53.246	292.265	292.265	0.	−104.600	−125.138	21.924
300	53.377	292.595	292.266	0.099	−104.689	−125.265	21.811
350	56.661	301.076	292.929	2.852	−135.938	−126.969	18.949
400	59.453	308.830	294.439	5.756	−136.327	−125.661	16.410
450	61.805	315.972	296.440	8.790	−136.693	−124.305	14.429
500	63.795	322.590	298.728	11.931	−137.036	−122.910	12.840
600	66.971	334.516	303.721	18.477	−137.655	−120.025	10.449
700	69.410	345.030	308.886	25.301	−138.194	−117.043	8.734
800	71.355	354.430	314.002	32.342	−138.664	−113.989	7.443
900	72.944	362.929	318.974	39.560	−139.080	−110.879	6.435
1000	74.259	370.685	323.763	46.922	−139.456	−107.725	5.627
1100	75.357	377.815	328.357	54.405	−139.806	−104.535	4.964
1200	76.281	384.413	332.757	61.988	−140.142	−101.313	4.410
1300	77.063	390.550	336.969	69.656	−140.477	−98.064	3.940
1400	77.728	396.286	341.003	77.396	−140.817	−94.789	3.537
1500	78.296	401.669	344.870	85.198	−141.173	−91.489	3.186
1600	78.785	406.738	348.580	93.053	−141.549	−88.165	2.878
1700	79.207	411.527	352.143	100.953	−141.953	−84.816	2.606
1800	79.573	416.065	355.569	108.893	−142.389	−81.443	2.363
1900	79.893	420.376	358.868	116.866	−142.862	−78.044	2.146
2000	80.174	424.482	362.047	124.870	−143.376	−74.619	1.949
2100	80.420	428.399	365.114	132.900	−143.936	−71.168	1.770
2200	80.639	432.146	368.076	140.953	−144.543	−67.689	1.607
2300	80.833	435.735	370.940	149.027	−145.201	−64.181	1.458
2400	81.006	439.179	373.712	157.119	−196.170	−59.574	1.297
2500	81.160	442.489	376.398	165.227	−197.012	−53.865	1.125
2600	81.299	445.674	379.001	173.350	−197.876	−48.123	0.967
2700	81.424	448.745	381.528	181.487	−198.762	−42.346	0.819
2800	81.537	451.708	383.982	189.635	−199.671	−36.537	0.682
2900	81.640	454.571	386.367	197.794	−200.601	−30.694	0.553
3000	81.733	457.341	388.687	205.963	−201.551	−24.819	0.432
3100	81.818	460.022	390.945	214.140	−202.520	−18.912	0.319
3200	81.896	462.621	393.144	222.326	−203.506	−12.974	0.212
3300	81.967	465.142	395.288	230.519	−204.506	−7.004	0.111
3400	82.032	467.590	397.379	238.719	−205.520	−1.004	0.015
3500	82.092	469.969	399.419	246.925	−206.543	5.026	−0.075
3600	82.147	472.282	401.411	255.137	−207.574	11.086	−0.161
3700	82.199	474.534	403.357	263.355	−208.611	17.174	−0.242
3800	82.246	476.727	405.259	271.577	−209.651	23.290	−0.320
3900	82.290	478.864	407.119	279.804	−210.692	29.434	−0.394
4000	82.331	480.947	408.939	288.035	−211.731	35.604	−0.465
4100	82.369	482.981	410.720	296.270	−212.767	41.800	−0.533
4200	82.404	484.966	412.464	304.508	−693.648	55.046	−0.685
4300	82.437	486.906	414.173	312.751	−693.584	72.871	−0.885
4400	82.468	488.801	415.848	320.996	−693.515	90.695	−1.077
4500	82.497	490.655	417.489	329.244	−693.437	108.517	−1.260
4600	82.524	492.468	419.100	337.495	−693.351	126.337	−1.435
4700	82.550	494.243	420.680	345.749	−693.255	144.155	−1.602
4800	82.574	495.982	422.230	354.005	−693.149	161.972	−1.763
4900	82.596	497.684	423.753	362.264	−693.032	179.785	−1.917
5000	82.618	499.353	425.248	370.524	−692.903	197.597	−2.064
5100	82.638	500.989	426.718	378.787	−692.762	215.405	−2.206
5200	82.656	502.594	428.161	387.052	−692.610	233.211	−2.343
5300	82.674	504.169	429.581	395.318	−692.445	251.014	−2.474
5400	82.691	505.714	430.976	403.587	−692.269	268.813	−2.600
5500	82.707	507.232	432.349	411.857	−692.080	286.609	−2.722
5600	82.723	508.722	433.699	420.128	−691.878	304.402	−2.839
5700	82.737	510.187	435.029	428.401	−691.665	322.191	−2.953
5800	82.751	511.626	436.337	436.675	−691.440	339.976	−3.062
5900	82.764	513.040	437.625	444.951	−691.203	357.757	−3.167
6000	82.776	514.432	438.893	453.228	−690.954	375.533	−3.269

PREVIOUS: March 1966 (1 atm) CURRENT: March 1966 (1 bar)

Tribromoborane (BBr_3) LIQUID $M_r = 250.522$ Tribromoborane (BBr_3) $B_1Br_3(l)$

$S°(298.15\ K) = [228.9]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298.15\ K) = [-238.49 \pm 0.2]\ kJ{\cdot}mol^{-1}$

$T_{fus} = 228.9\ K$ $\Delta_{fus}H° =$ Unknown

Enthalpy of Formation

The enthalpy of formation of boron tribromide liquid has been determined by Skinner and Smith[1] by hydrolysis to H_3BO_3 and HBr. The adopted enthalpy of formation is calculated from the hydrolysis data[1] using $\Delta_fH°(H_3BO_3, cr, 298.15\ K)$ from these tables, $\Delta_{sol}H°(H_3BO_3, cr)$, from Fasilino[2] with the dilution data of Smisko and Mason.[3] The $\Delta_fH°(HBr, aq)$ was taken from Evans.[4]

Heat Capacity and Entropy

The heat capacity was estimated from that of the gas by Kelley.[5] The entropy is back calculated from that of the gas by adjusting the free energy functions to give the best fit of the vapor pressure data.

Fusion Data

The temperature of melting was reported by Boubeau and Keller,[6] and Stock and Kuss.[7] This value was recently confirmed by the triple point measurement of 227.31 K by Barber, Boynton, and Gallagher.[8]

Vaporization Data

The boiling point is from the data of Stock and Kuss.[7] A 2nd and 3rd law analysis of the vapor pressure data of Stock and Kuss[7] and Barber *et al.*[8] indicated that the data of Stock and Kuss[7] gave the best agreement as indicated below.

Sources	2nd law	$\Delta_{vap}H°(298.15\ K)$, $kcal{\cdot}mol^{-1}$ 3rd law $S°(298.15\ K) = 54.7$	 $S°(298.15\ K) = 54.26$
7	8.175 ± 0.03	8.222 (−0.02)	8.361 (0.42)
8	8.229 ± 0.03	8.203 (−0.44)	8.347 (0.00)

Stock and Kuss[7] had the first eight data points rejected due to a statistical test on the 3rd law values. The values in parentheses are values of the 3rd law drift measured as $\Delta(\Delta H)/\Delta T$. The 2nd law entropy also confirmed the choice of the data of Stock and Kuss[7] and an entropy of $54.7\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$.

References

[1] H. A. Skinner and N. B. Smith, Trans. Faraday Soc. **51**, 19 (1955).
[2] L. G. Fasilino, National Research Corporation, Special Report NONR 3608(00), (June 2, 1964).
[3] J. Smisko and L. S. Mason, J. Am. Chem. Soc. **72**, 3679 (1950).
[4] W. H. Evans, U. S. Nat. Bur. Stand. Report 8504, Appendix III, (1964).
[5] K. K. Kelley, U. S. Bur. Mines Bull. 383, 166 pp. (1935).
[6] J. Goubeau and H. Keller, Z. anorg. allgem. Chem. **267**, 1 (1951).
[7] A. Stock and E. Kuss, Ber. **47**, 3113 (1914).
[8] W. F. Barber, C. F. Boynton and P. E. Gallagher, J. Chem. Eng. Data **9**, 137 (1964).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200	128.030	177.745	240.576	−12.566	−224.975	−233.814	61.066
298.15	128.030	228.865	228.865	0.	−238.488	−236.914	41.506
300	128.030	229.657	228.867	0.237	−238.482	−236.904	41.249
400	128.030	266.489	233.889	13.040	−278.762	−227.783	29.745
500	128.030	295.058	243.372	25.843	−273.227	−215.687	22.533
600	128.030	318.400	253.990	38.646	−267.984	−204.675	17.819
700	128.030	338.136	264.638	51.449	−262.944	−194.524	14.516
800	128.030	355.233	274.917	64.252	−258.053	−185.085	12.085
900	128.030	370.312	284.696	77.055	−253.277	−176.252	10.229
1000	128.030	383.802	293.944	89.858	−248.598	−167.946	8.773

PREVIOUS: September 1962   CURRENT: December 1964

Tribromoborane (BBr$_3$) IDEAL GAS $M_r = 250.522$ Tribromoborane (BBr$_3$) B$_1$Br$_3$(g)

$S°(298.15\ K) = 324.31\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = -181.9 \pm 0.2\ kJ \cdot mol^{-1}$

$\Delta_f H°(298.15\ K) = -204.2 \pm 0.2\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}
278(1)
379(1)
827(2)
150(2)

Ground State Quantum Weight: [1] $\sigma = 6$
Point Group: D$_{3h}$
Bond Distance: B–Br = 1.87 ± 0.02 Å
Bond Angle: Br–B = 120° ± 6°
Product of the Moments of Inertia: $I_A I_B I_C = 6.742600 \times 10^{-112}\ g^3 \cdot cm^6$

Enthalpy of Formation

$\Delta_f H°(298.15\ K)$ is obtained from the enthalpy of formation of the liquid plus the heat of vaporization at 298.15 K, taken as 8.20 kcal·mol^{-1} as the average 2nd and 3rd law value derived from the vapor pressures of Stock and Kuss.[1] Refer to BBr$_3$(l) table for details.

Heat Capacity and Entropy

Vibrational frequencies were obtained from Wentink and Tiensuu[2] and modified for the natural isotopic abundance (^{10}B 18.83%, ^{11}B 81.1%). B–Br bond distance was reported by Wentink and Tiensuu.[2] Br–B–Br angle was taken from Sutton.[3] The principal moments of inertia are $I_A = I_B = 69.5984 \times 10^{-39}$, $I_C = 139.1968 \times 10^{-39}\ g \cdot cm^2$.

References

[1] A. Stock and E. Kuss, Ber. 47, 3113 (1914).
[2] T. Wentink, Jr., and V. H. Tiensuu, J. Chem. Phys. 28, 825 (1958).
[3] L. E. Sutton, Ed., "Tables of Interatomic Distances and Configuration in Molecules and Ions", Special Publication No. 11, The Chemical Society, London, (1958).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−15.711	−181.912	−181.912	INFINITE
100	48.309	260.958	379.306	−11.835	−182.250	−200.238	104.593
200	60.557	298.686	330.295	−6.322	−184.421	−217.449	56.792
250	64.597	312.649	325.406	−3.189	−185.884	−225.543	47.125
298.15	67.771	324.307	324.307	0.	−204.179	−231.062	40.481
300	67.880	324.727	324.309	0.125	−204.285	−231.228	40.260
350	70.521	335.397	325.145	3.588	−250.425	−233.188	34.801
400	72.626	344.956	327.034	7.169	−250.324	−230.733	30.131
450	74.301	353.611	329.514	10.843	−250.239	−228.289	26.499
500	75.640	361.511	332.325	14.593	−250.168	−225.854	23.595
600	77.590	375.487	338.384	22.261	−250.060	−221.002	19.240
700	78.897	387.552	344.566	30.090	−249.994	−216.165	16.130
800	79.804	398.150	350.615	38.028	−249.968	−211.335	13.799
900	80.455	407.589	356.431	46.042	−249.981	−206.505	11.985
1000	80.936	416.092	361.979	54.113	−250.034	−201.672	10.534
1100	81.301	423.824	367.255	62.226	−250.126	−196.832	9.347
1200	81.583	430.910	372.268	70.370	−250.258	−191.981	8.357
1300	81.806	437.450	377.034	78.540	−250.430	−187.118	7.518
1400	81.985	443.519	381.569	86.730	−250.644	−182.240	6.799
1500	82.130	449.180	385.889	94.936	−250.901	−177.346	6.176
1600	82.250	454.485	390.013	103.155	−251.202	−172.432	5.629
1700	82.350	459.474	393.953	111.386	−251.549	−167.499	5.147
1800	82.434	464 184	397.725	119.625	−251.946	−162.544	4.717
1900	82.506	468.643	401.342	127.872	−252.393	−157.565	4.332
2000	82.567	472.876	404.813	136.126	−252.895	−152.561	3.984
2100	82.620	476.906	408.151	144.385	−253.454	−147.531	3.670
2200	82.666	480.751	411.364	152.649	−254.073	−142.472	3.383
2300	82.706	484.426	414.462	160.918	−254.753	−137.385	3.120
2400	82.742	487.947	417.451	169.191	−305.756	−131.197	2.855
2500	82.773	491.325	420.339	177.466	−306.640	−123.906	2.589
2600	82.801	494.572	423.132	185.745	−307.556	−116.579	2.342
2700	82.825	497.697	425.836	194.026	−308.503	−109.215	2.113
2800	82.848	500.710	428.457	202.310	−309.480	−101.817	1.899
2900	82.867	503.618	430.998	210.596	−310.484	−94.382	1.700
3000	82.885	506.427	433.466	218.883	−311.515	−86.913	1.513
3100	82.902	509.145	435.864	227.173	−312.568	−79.409	1.338
3200	82.917	511.778	438.195	235.464	−313.640	−71.871	1.173
3300	82.930	514.329	440.464	243.756	−314.729	−64.298	1.018
3400	82.942	516.805	442.673	252.050	−315.829	−56.693	0.871
3500	82.954	519.210	444.826	260.344	−316.938	−49.056	0.732
3600	82.964	521.547	446.924	268.640	−318.051	−41.386	0.600
3700	82.974	523.820	448.972	276.937	−319.164	−33.685	0.476
3800	82.982	526.033	450.971	285.235	−320.273	−25.955	0.357
3900	82.991	528.188	452.923	293.534	−321.376	−18.196	0.244
4000	82.998	530.290	454.831	301.833	−322.468	−10.408	0.136
4100	83.005	532.339	456.697	310.133	−323.546	−2.593	0.033
4200	83.012	534.340	458.522	318.434	−804.457	12.272	−0.153
4300	83.018	536.293	460.308	326.736	−804.412	31.718	−0.385
4400	83.023	538.202	462.057	335.038	−804.347	51.162	−0.607
4500	83.029	540.067	463.769	343.340	−804.260	70.604	−0.820
4600	83.034	541.892	465.448	351.644	−804.150	90.045	−1.022
4700	83.038	543.678	467.094	359.947	−804.014	109.482	−1.217
4800	83.043	545.426	468.707	368.251	−803.853	128.917	−1.403
4900	83.047	547.139	470.291	376.556	−803.664	148.347	−1.581
5000	83.051	548.816	471.844	384.860	−803.448	167.774	−1.753
5100	83.054	550 461	473.370	393.166	−803.203	187.197	−1.917
5200	83.058	552.074	474.868	401.471	−802.931	206.613	−2.075
5300	83.061	553.656	476.340	409.777	−802.630	226.025	−2.228
5400	83.064	555.209	477.786	418.083	−802.301	245.431	−2.374
5500	83 067	556.733	479.207	426.390	−801.943	264.830	−2.515
5600	83.070	558.230	480.605	434.697	−801.559	284.222	−2.651
5700	83.072	559.700	481.980	443.004	−801.147	303.608	−2.782
5800	83.075	561.145	483.332	451.311	−800.708	322.985	−2.909
5900	83.077	562.565	484.663	459.619	−800.244	342.355	−3.031
6000	83.079	563.961	485.973	467.927	−799.755	361.717	−3.149

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Tribromoborane (BBr$_3$) B$_1$Br$_3$(g)

Chloroborane (BCl) IDEAL GAS $M_r = 46.263$ Chloroborane (BCl) $B_1Cl_1(g)$

$S°(298.15\ K) = 213.24\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 138.4\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 141.4\ kJ·mol^{-1}$

Electronic Level and Quantum Weight		
State	ϵ_i, cm^{-1}	g_i
$^1\Sigma^+$	0	1

$\omega_e = 843.65\ cm^{-1}$ $\omega_e x_e = 5.167\ cm^{-1}$ $\sigma = 1$
$B_e = 0.6914\ cm^{-1}$ $\alpha_e = 0.00657\ cm^{-1}$ $r_e = 1.7157$ Å

Enthalpy of Formation

Dissociation energies of BCl(g) has been reported by Herzberg,[1] Gaydon,[2] and Barrow [3] The corresponding values of $\Delta_f H°$(BCl, g, 298.15 K) are derived. The results are given as follows:

Source	Dissociation Energy, D_0° eV	kcal·mol^{-1}	$\Delta_f H°$(298.15 K) kcal·mol^{-1}
1	4.2	96.9	62.6
2	5.1 ± 0.4	117.6 ± 9.2	41.8 ± 9.2
3	—	127	33.8 ± 4

The last value of $\Delta_f H°$(298.15 K) listed in the above table is adopted. Using the bond energy, D_0°(B–Cl), obtained from $BCl_3(g)$ molecule, $\Delta_f H°$(298 15 K) for BCl(g) is calculated as 37.8 kcal·mol^{-1} employing the same ratio of *D_0°(B–X)/ average bond energy of BX_3 as found in* BF(g) and $BF_3(g)$, which is within the uncertainty of the value evaluated from dissociation energy.

Heat Capacity and Entropy

The spectroscopic constants are obtained from Herzberg[1] and corrected to the average isotopic species.

References

[1] G. Herzberg, Spectra of Diatomic Molecules, D. Van Nostrand Company, Inc., New York, (1950).
[2] A. G. Gaydon, "*Dissociation Energies and Spectra of Diatomic Molecules*," 2nd ed., Chapman and Hall Ltd., London, 261 pp. (1953).
[3] R. F. Barrow, Trans. Faraday Soc. 56, 952 (1960).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	-8.862	138.362	138.362	INFINITE
100	29.117	180.668	240.206	-5.954	139.790	131.204	-68.534
200	29.874	200.994	216.081	-3.017	140.875	122.156	-31.904
250	30.748	207.751	213.761	-1.502	141.209	117.435	-24.537
298.15	31.659	213.245	213.245	0.	141.419	112.835	-19.768
300	31.693	213.441	213.245	0.059	141.425	112.658	-19.615
350	32.572	218.394	213.635	1.666	141.546	107.852	-16.096
400	33.335	222.794	214.510	3.314	141.583	103.036	-13.455
450	33.976	226.759	215.654	4.997	141.551	98.219	-11.401
500	34.510	230.367	216.948	6.710	141.462	93.408	-9.758
600	35.322	236.735	219.729	10.204	141.159	83.823	-7.297
700	35.892	242.225	222.560	13.766	140.730	74.300	-5.544
800	36.307	247.046	225.325	17.377	140.209	64.844	-4.234
900	36.619	251.342	227.982	21.024	139.614	55.459	-3.219
1000	36.861	255.213	230.514	24.698	138.958	46.143	-2.410
1100	37.054	258.735	232.922	28.394	138.249	36.895	-1.752
1200	37.214	261.967	235.210	32.108	137.493	27.714	-1.206
1300	37.348	264.951	237.384	35.836	136.693	18.598	-0.747
1400	37.464	267.723	239.453	39.577	135.853	9.545	-0.356
1500	37.566	270.311	241.425	43.329	134.975	0.554	-0.019
1600	37.656	272.738	243.307	47.090	134.060	-8.378	0.274
1700	37.739	275.024	245.106	50.860	133.109	-17.251	0.530
1800	37.814	277.183	246.829	54.637	132.124	-26.068	0.756
1900	37.884	279.230	248.481	58.422	131.103	-34.829	0.958
2000	37.950	281.174	250.067	62.214	130.049	-43.535	1.137
2100	38.012	283.028	251.593	66.012	128.960	-52.187	1.298
2200	38.071	284.797	253.063	69.816	127.837	-60.787	1.443
2300	38.128	286.491	254.479	73.626	126 679	-69.335	1.575
2400	38.182	288.115	255.847	77.442	75.227	-76.763	1.671
2500	38.235	289.674	257.169	81.263	73.920	-83.069	1.736
2600	38.286	291.175	258.449	85.089	72.611	-89.323	1.795
2700	38.336	292.621	259.688	88.920	71.297	-95.526	1.848
2800	38.385	294.016	260.889	92.756	69.978	-101 681	1.897
2900	38.433	295.364	262.055	96.597	68.655	-107.788	1.941
3000	38.480	296.668	263.187	100.443	67.327	-113.850	1.982
3100	38.527	297.930	264.287	104.293	65.994	-119.867	2.020
3200	38.572	299.154	265.358	108.148	64.656	-125.841	2.054
3300	38.617	300.342	266.400	112.008	63.313	-131.774	2.086
3400	38.662	301.495	267.415	115.872	61.967	-137.665	2.115
3500	38.706	302.617	268.405	119.740	60.618	-143.517	2.142
3600	38.750	303.708	269.371	123.613	59.266	-149.330	2.167
3700	38.793	304.770	270.313	127.490	57.913	-155.106	2.190
3800	38.837	305.805	271.234	131.372	56.560	-160.845	2.211
3900	38.879	306.814	272.133	135.257	55.208	-166.549	2.231
4000	38.922	307.799	273.012	139.147	53.859	-172.218	2.249
4100	38.964	308.761	273.873	143.042	52.513	-177.853	2.266
4200	39.006	309.700	274.714	146.940	-428.678	-176.431	2.194
4300	39.048	310.619	275.539	150.843	-428.926	-170.422	2.070
4400	39.090	311.517	276.346	154.750	-429.168	-164.408	1.952
4500	39.131	312.396	277.138	158.661	-429 404	-158.388	1.839
4600	39.173	313.256	277.914	162.576	-429.632	-152.363	1.730
4700	39.214	314.099	278.675	166.495	-429.852	-146.333	1.626
4800	39.255	314.925	279.421	170.419	-430.063	-140.298	1.527
4900	39.296	315.735	280.154	174.346	-430.264	-134.259	1.431
5000	39.337	316.529	280.874	178.278	-430.455	-128.217	1.339
5100	39.378	317.309	281.580	182.214	-430.635	-122.170	1.251
5200	39.419	318.074	282.275	186.154	-430.803	-116.120	1.166
5300	39.459	318.825	282.957	190.098	-430.960	-110.067	1.085
5400	39.500	319.563	283.629	194.046	-431.106	-104 011	1.006
5500	39.541	320.288	284.288	197.998	-431.239	-97.952	0.930
5600	39.581	321.001	284.938	201.954	-431.359	-91.892	0.857
5700	39.621	321.702	285.577	205.914	-431.468	-85.829	0.787
5800	39.662	322.391	286.205	209.878	-431.565	-79.764	0.718
5900	39.702	323.070	286.824	213.846	-431.650	-73.698	0.652
6000	39.742	323.737	287 434	217.818	-431.723	-67.630	0.589

PREVIOUS: December 1964 (*1 atm*) CURRENT: December 1964 (1 bar)

Chloroborane (BCl) $B_1Cl_1(g)$

Chloroborane, Ion (BCl^+) IDEAL GAS $M_r = 46.26245$ Chloroborane, Ion (BCl^+) $B_1Cl_1^+(g)$

$\Delta_f H°(0\ K) = [1225 \pm 42]\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = [219.1 \pm 2]\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = [1234 \pm 42]\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$[^2\Sigma]$	0	[2]
	[2800]	[4]

$\omega_e = [845]\ cm^{-1}$ $\omega_e x_e = [5]\ cm^{-1}$ $\sigma = 1$

$B_e = [0\ 68]\ cm^{-1}$ $\alpha_e = [0.0056]\ cm^{-1}$ $r_e = [1.73]$ Å

Enthalpy of Formation

Several values of the appearance potential of BCl^+ from BCl_3 have been reported. Osberghaus[1] gave 19.2 eV, Marriott and Craggs[2] reported 18.54 ± 0.07 eV, and Koski *et al.*[3] obtained two values of 17.2 ± 0.2 Ev and 20 ± 0.2 eV. We make the presumption that the higher values, 19.2 and 20, refer to the reaction $BCl_3(g) + e^-$, $2\ Cl(g) + 2e^-$ and the other values to $BCl_3(g) + e^- \rightarrow BCl^+ + Cl_2(g) + 2\ e^-$. Using the lower value in each case to help eliminate any excess kinetic energy, we obtain $\Delta_f H°(BCl^+, g, 298.15\ K) = 289$ and $300\ kcal \cdot mol^{-1}$, respectively. We adopt an average value of $\Delta_f H°(BCl^+, g, 298.15\ K) = 295 \pm 10\ kcal \cdot mol^{-1}$, which corresponds to an ionization potential for BCl(g) of 11.3 ± 0.3 eV.

Heat Capacity and Entropy

BCl^+ is isoelectronic with BeCl, and the ground state configuration and electronic levels are estimated by comparison with BeCl. The bond length, frequency and anharmonicity constant are estimated between the value for BCl and BeCl; the rotational constant is calculated from the bond length and atomic masses, and α_e is obtained from the above constants assuming a Morse potential function.

References

[1] O. Osberghaus, Z. Phys. 128, 366 (1950).

[2] J. Marriott and J. D. Craggs, J. Electron. Contr. 3, 194 (1957).

[3] W. S. Koski, J. J. Kaufman and C. F. Pachuki, J Am. Chem. Soc. 81, 1326 (1959).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8.860	1225.027		
100	29.117	186.560	246.084	−5.952			
200	29.867	206.884	221.965	−3.016			
250	30.736	213.639	219.647	−1.502			
298.15	31.643	219.131	219.131	0.	1234.280	1197.686	−209.830
300	31.678	219.326	219.131	0.059	1234.325	1197.459	−208.496
350	32.555	224.277	219.520	1.665	1235.484	1191.222	−177.780
400	33.316	228.675	220.395	3.312	1236.559	1184.825	−154.722
450	33.957	232.637	221.538	4.994	1237.565	1178.297	−136.773
500	34 490	236.243	222.831	6.706	1238.515	1171.660	−122.402
600	35.300	242.608	225.611	10.198	1240.288	1158.120	−100.823
700	35.869	248.094	228.440	13.758	1241.936	1144.294	−85.388
800	36.282	252.912	231.204	17.367	1243.491	1130.238	−73.797
900	36.592	257.205	233.859	21.011	1244.972	1115.991	−64.770
1000	36.832	261.073	236.390	24.683	1246.391	1101.584	−57.541
1100	37.024	264.593	238.796	28.376	1247.758	1087.036	−51.619
1200	37.181	267.821	241.082	32.086	1249 077	1072.367	−46 679
1300	37.313	270.803	243.255	35.811	1250.353	1057.589	−42.494
1400	37.426	273.572	245.323	39.548	1251.588	1042.714	−38.904
1500	37.526	276.158	247.294	43.296	1252.785	1027.752	−35.790
1600	37.614	278.582	249.174	47.053	1253.944	1012.712	−33.062
1700	37.694	280.865	250.972	50.819	1255.068	997.601	−30.653
1800	37.767	283.022	252.693	54.592	1256.156	982.424	−28.509
1900	37.835	285.065	254.343	58.372	1257.210	967.188	−26.590
2000	37.898	287.008	255.929	62.158	1258.229	951.897	−24.861
2100	37.957	288.858	257.453	65.951	1259.213	936.556	−23.296
2200	38.014	290.625	258.921	69.750	1260.163	921.169	−21.871
2300	38.068	292.316	260.336	73.554	1261.078	905.739	−20.570
2400	38.120	293.938	261.703	77.363	1211.698	891.340	−19.400
2500	38.171	295.495	263.024	81.178	1212.464	877.976	−18.344
2600	38.220	296.993	264.302	84.997	1213.226	864.581	−17.370
2700	38.268	298.436	265.539	88.822	1213.984	851.157	−16.467
2800	38.315	299.829	266.739	92.651	1214.738	837.706	−15.628
2900	38.361	301.174	267.903	96.485	1215.486	824.227	−14.846
3000	38.407	302.475	269.034	100.323	1216.229	810.723	−14.116
3100	38.453	303.735	270.133	104.166	1216.967	797.193	−13.433
3200	38.499	304.957	271.203	108.014	1217.700	783.641	−12.792
3300	38.545	306.142	272.244	111.866	1218.429	770.065	−12.189
3400	38.591	307.294	273.258	115.723	1219.154	756.467	−11.622
3500	38.638	308.413	274.246	119.584	1219.876	742.848	−11.086
3600	38.686	309.502	275.210	123.450	1220.597	729.209	−10.581
3700	38.735	310.563	276.152	127.321	1221.316	715.549	−10.102
3800	38.785	311.597	277.071	131.197	1222.037	701.870	−9.648
3900	38.837	312.605	277.969	135.079	1222.759	688.172	−9.217
4000	38.890	313.589	278.847	138.965	1223.484	674.456	−8.807
4100	38.945	314.550	279.706	142.857	1224.214	660.721	−8.418
4200	39.002	315.489	280.547	146.754	745.101	653.993	−8.134
4300	39.062	316.407	281.371	150.657	746.932	651.802	−7.918
4400	39.124	317.306	282.177	154.566	748.770	649.568	−7 711
4500	39.188	318.186	282.968	158.482	750.618	647.293	−7.514
4600	39.255	319.048	283.743	162.404	752.475	644.976	−7.324
4700	39.324	319.893	284.503	166.333	754.343	642.619	−7.142
4800	39.397	320.721	285.249	170.269	756.223	640.222	−6.967
4900	39.472	321.535	285.981	174.213	758.117	637.786	−6.799
5000	39.550	322.333	286.700	178.164	760.024	635.311	−6.637
5100	39.631	323.117	287.406	182.123	761.946	632.798	−6.481
5200	39.715	323.887	288.101	186.090	763.883	630.246	−6.331
5300	39.802	324 644	288.783	190.066	765.837	627.658	−6.186
5400	39.892	325.389	289.454	194.051	767.807	625.032	−6.046
5500	39.985	326.122	290.114	198.044	769.795	622.370	−5.911
5600	40.081	326.843	290.764	202.048	771.800	619.671	−5.780
5700	40.180	327.554	291.403	206.061	773.822	616.937	−5.654
5800	40.282	328.253	292.032	210.084	775.863	614.167	−5.531
5900	40.386	328.943	292.652	214.117	777.922	611.361	−5.413
6000	40.493	329.623	293.262	218.161	780.000	608.520	−5.298

PREVIOUS: June 1968 (1 atm) CURRENT: June 1968 (1 bar)

Chloroborane, Ion (BCl^+) $B_1Cl_1^+(g)$

Chlorofluoroborane (BClF) IDEAL GAS $M_r = 65.261403$ Chlorofluoroborane (BClF) $B_1Cl_1F_1(g)$

$\Delta_fH°(0\ K) = [-315 \pm 29]\ kJ\cdot mol^{-1}$

$S°(298.15\ K) = [264.65]\ J\cdot K^{-1}\cdot mol^{-1}$ $\Delta_fH°(298.15\ K) = [-314 \pm 29]\ kJ\cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[920](1)
[360](1)
[1220](1)

Ground State Quantum Weight: [2] $\sigma = 1$

Point Group: C_s

Bond Distances: B–Cl = [1.73] Å; B–F = [1.295] Å

Bond Angle: F–B–Cl = [120]°

Product of the Moments of Inertia: $I_AI_BI_C = [1.811033 \times 10^{-115}]\ g^3\ cm^6$

Enthalpy of Formation

The value of $\Delta_fH°(298.15\ K)$ for BClF(g) is estimated based on an assumption that $\Delta_rH° = 0$ for the reaction $BCl_2(g) + BF_2(g) = 2\ BClF(g)$. The values of $\Delta_fH°(298.15\ K)$ of $BCl_2(g)$ and $BF_2(g)$, used for calculation, are −20 and −130 kcal·mol^{-1}, respectively.

Heat Capacity and Entropy

The ground state quantum weight and bond angle are assumed to be the same as those for $BF_2(g)$. The bond distances of B–Cl and B–F are estimated by comparison with those in $BCl_3(g)$ and $BF_3(g)$ molecules, respectively. The vibrational frequencies were estimated from the corresponding values for $BCl_2(g)$ and $BF_2(g)$. The principal moments of inertia are: $I_A = 0.7794 \times 10^{-39}$, $I_B = 14.8586 \times 10^{-39}$, and $I_C = 15.6380 \times 10^{-39}\ g\ cm^2$.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−11.008	−314.591	−314.591	INFINITE
100	34.530	223.216	299.791	−7.657	−314.174	−318.496	166.365
200	38.735	248.470	268.419	−3.990	−313.823	−322.971	84.351
250	40.690	257.324	265.340	−2.004	−313.769	−325.267	67.961
298.15	42.547	264.650	264.650	0.	−313.800	−327.480	57.373
300	42.617	264.913	264.651	0.079	−313.803	−327.564	57.034
350	44.450	271.622	265.176	2.256	−313.906	−329.851	49.228
400	46.125	277.669	266.366	4.521	−314.067	−332.118	43.370
450	47.610	283.189	267.933	6.865	−314.273	−334.363	38.812
500	48.901	288.274	269.716	9.279	−314.509	−336.582	35.163
600	50.964	297.382	273.586	14.277	−315.045	−340.948	29.682
700	52.475	305.357	277.567	19.453	−315.636	−345.219	25.761
800	53.590	312.441	281.492	24.759	−316.267	−349.402	22.814
900	54.425	318.803	285.290	30.162	−316.933	−353.505	20.517
1000	55.061	324.572	288.934	35.638	−317.633	−357.531	18.676
1100	55.554	329.844	292.417	41.169	−318.366	−361.486	17.166
1200	55.942	334.695	295.741	46.745	−319.134	−365.372	15.904
1300	56.253	339.185	298.912	52.355	−319.936	−369.193	14.834
1400	56.505	343.364	301.940	57.994	−320.773	−372.951	13.915
1500	56.712	347.270	304.833	63.655	−321.647	−376.648	13.116
1600	56.884	350.935	307.601	69.335	−322.557	−380.285	12.415
1700	57.028	354.388	310.253	75.031	−323.505	−383.864	11.795
1800	57.150	357.652	312.796	80.740	−324.489	−387.386	11.242
1900	57.254	360.744	315.239	86.460	−325.510	−390.853	10.745
2000	57.344	363.683	317.588	92.190	−326.566	−394.265	10.297
2100	57.421	366.483	319.851	97.929	−327.658	−397.623	9.890
2200	57.489	369.156	322.031	103.674	−328.785	−400.928	9.519
2300	57.548	371.713	324.136	109.426	−329.945	−404.182	9.179
2400	57.600	374.163	326.170	115.183	−381.397	−406.315	8.843
2500	57.646	376.516	328.137	120.946	−382.699	−407.327	8.511
2600	57.687	378.777	330.042	126.713	−384.000	−408.286	8.203
2700	57.724	380.955	331.887	132.483	−385.297	−409.195	7.916
2800	57.757	383.055	333.677	138.257	−386.592	−410.057	7.650
2900	57.787	385.082	335.415	144.034	−387.881	−410.872	7.401
3000	57.813	387.042	337.104	149.815	−389.166	−411.643	7.167
3100	57.838	388.938	338.745	155.597	−390.444	−412.371	6.948
3200	57.860	390.775	340.343	161.382	−391.715	−413.058	6.742
3300	57.880	392.555	341.898	167.169	−392.978	−413.705	6.548
3400	57.898	394.283	343.413	172.958	−394.231	−414.315	6.365
3500	57.915	395.962	344.891	178.749	−395.474	−414.887	6.192
3600	57.931	397.594	346.332	184.541	−396.706	−415.424	6.028
3700	57.945	399.181	347.739	190.335	−397.924	−415.928	5.872
3800	57.958	400.727	349.114	196.130	−399.129	−416.398	5.724
3900	57.970	402.232	350.456	201.926	−400.318	−416.837	5.583
4000	57.982	403.700	351.769	207.724	−401.492	−417.246	5.449
4100	57.992	405.132	353.053	213.523	−402.647	−417.625	5.321
4200	58.002	406.530	354.310	219.322	−883.634	−410.952	5.111
4300	58.011	407.895	355.540	225.123	−883.665	−399.698	4.855
4400	58.019	409.228	356.745	230.924	−883.677	−388.443	4.611
4500	58.027	410.532	357.926	236.727	−883.670	−377.187	4.378
4600	58.035	411.808	359.084	242.530	−883.643	−365.932	4.155
4700	58.042	413.056	360.219	248.334	−883.595	−354.678	3.942
4800	58.048	414.278	361.332	254.138	−883.527	−343.425	3.737
4900	58.054	415.475	362.425	259.943	−883.438	−332.174	3.541
5000	58.060	416.648	363.498	265.749	−883.328	−320.925	3.353
5100	58.066	417.798	364.551	271.555	−883.196	−309.678	3.172
5200	58.071	418.925	365.586	277.362	−883.044	−298.434	2.998
5300	58.076	420.031	366.603	283.170	−882.870	−287.193	2.830
5400	58.080	421.117	367.603	288.977	−882.674	−275.956	2.669
5500	58.084	422.183	368.585	294.786	−882.459	−264.722	2.514
5600	58.089	423.229	369.552	300.594	−882.222	−253.493	2.364
5700	58.092	424.258	370.503	306.403	−881.966	−242.268	2.220
5800	58.096	425.268	371.438	312.213	−881.689	−231.048	2.081
5900	58.100	426.261	372.359	318.023	−881.394	−219.832	1.946
6000	58.103	427.238	373.265	323.833	−881.079	−208.622	1.816

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Chlorodifluoroborane (BClF$_2$) IDEAL GAS M_r = 84.259806 Chlorodifluoroborane (BClF$_2$) B$_1$Cl$_1$F$_2$(g)

$S°(298.15 \text{ K}) = 274.83 \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = -883.0 \pm 20 \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = -885.3 \pm 20 \text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}	υ, cm^{-1}
1250(1)	1430(1)
697(1)	366(1)
429(1)	608(1)

Ground State Quantum Weight: 1 σ = 2
Point Group: C_{2v}
Bond Distances: B–Cl = [1.73] Å; B–F = [1.295] Å
Bond Angles: F–B–Cl = [120]°; F–B–F = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = [3.568886 \times 10^{-114}] \text{ g}^3\text{·cm}^6$

Enthalpy of Formation

The values for BCl$_2$F and BClF$_2$ of $\Delta_f H°(298.15 \text{ K}) = -154$ and $\Delta_f H°(298.15 \text{ K}) = -211$ 6 kcal·mol^{-1}, respectively, are obtained from the average bond energies of BF$_3$ and BCl$_3$. The calculated values are each made less negative by about 0.8 kcal·mol^{-1} in order to make them consistent with the equilibrium measurements of Higgins, Leisegang, Raw and Rossow[2] and Gunn and Sanborn[2] for the reaction $BF_3(g) + BCl_3(g) \rightarrow BClF_2(g) + BCl_2F(g)$. Values for the heat of reaction are $\Delta_r H°(298.15 \text{ K}) = +1.68$ kcal·mol^{-1} and $\Delta_r H°(298.15 \text{ K}) = 1.1$ (uncertainty of 0.5 to + 0.8) kcal·mol^{-1}, the former calculated from the measured equilibrium constant and the statistical entropy change and the latter obtained from the variation of the equilibrium constant with temperature. Selection of $\Delta_r H°(298.15 \text{ K}) = 1.6$ kcal·mol^{-1} fixes the sum of the enthalpy of formation of BClF$_2$ and BCl$_2$F as −365.6 kcal·mol^{-1}, but it does not determine the individual values. Thus, the selected enthalpies of formation are only as accurate as the average bond energy calculations on which they are based. A reasonable estimate of the uncertainty would be ± 5 kcal·mol^{-1}.

Heat Capacity and Entropy

The observed frequencies of Lindeman and Wilson[3] were adjusted to the normal isotopic composition of 81.2% ^{10}B and 18.8% ^{11}B. The bond angles are assumed to be 120° and the bond lengths are taken to be the same as in the respective trihalides. The principal moments of inertia are. $I_A = 7.9360 \times 10^{-39}$, $I_B = 17.6063 \times 10^{-39}$, and $I_C = 25.5423 \times 10^{-39}$ g·cm^2.

References

[1] T. H. S. Higgins, E. C. Leisegang, C J. G. Raw, and A. J. Rossouw, J. Chem. Phys. 23, 1544 (1955).
[2] S. R. Gunn and R. H. Sanborn, J. Chem. Phys. 33, 955 (1960).
[3] L. P. Lindeman and M. K. Wilson, J. Chem. Phys. 24, 242 (1956).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	S°	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−12.320	−883.026	−883.026	INFINITE
100	35.262	227.389	316.986	−8.960	−884.052	−880.272	459.807
200	45.615	254.879	279.545	−4.933	−884.806	−876.171	228.832
250	50.457	265.591	275.705	−2.528	−885.084	−873.980	182.608
298.15	54.466	274.830	274.830	0.	−885.334	−871.818	152.739
300	54 609	275.167	274.831	0.101	−885.344	−871.734	151.782
350	58.172	283.860	275.509	2.923	−885.597	−869.446	129.758
400	61.242	291.833	277.058	5.910	−885.852	−867.121	113.234
450	63.887	299.203	279.115	9.040	−886.105	−864.765	100.379
500	66.163	306.055	281.470	12.292	−886.351	−862.381	90.092
600	69.800	318.456	286.623	19.100	−886.815	−857.542	74 656
700	72.492	329.428	291.970	26.221	−887.236	−852.630	63.624
800	74.504	339.246	297.276	33.576	−887.624	−847.659	55.346
900	76.027	348.113	302.440	41.106	−887.990	−842.641	48.906
1000	77.199	356.187	307.417	48.769	−888.347	−837.583	43.751
1100	78.114	363.589	312.192	56.537	−888.704	−832.490	39.532
1200	78.840	370.418	316.763	64.386	−889.071	−827.363	36.014
1300	79.424	376.753	321.137	72.300	−889.453	−822.206	33.037
1400	79.899	382.657	325.323	80.267	−889.858	−817.018	30.483
1500	80.290	388.183	329.331	88.277	−890.288	−811.800	28.269
1600	80.616	393.375	333.174	96.323	−890.747	−806.553	26.331
1700	80.891	398.271	336.860	104.399	−891.237	−801.276	24.620
1800	81.123	402.902	340.402	112.500	−891.759	−795.969	23.098
1900	81.322	407.293	343.808	120.622	−892.314	−790.632	21.736
2000	81 493	411.469	347.087	128.763	−892.900	−785.266	20.509
2100	81.641	415.449	350.249	136.920	−893.517	−779.869	19.398
2200	81.771	419.250	353.299	145.091	−894.163	−774.442	18.388
2300	81.884	422.887	356.246	153.274	−894.837	−768.985	17.464
2400	81.984	426.374	359.096	161.467	−945.794	−762.430	16.594
2500	82.073	429.723	361.855	169.670	−946.593	−754.773	15.770
2600	82.152	432.943	364.527	177.881	−947.380	−747.084	15.009
2700	82.223	436.045	367.119	186.100	−948.153	−739.366	14.304
2800	82.286	439.036	369.634	194.326	−948.909	−731.619	13.649
2900	82.343	441.925	372.078	202.557	−949.648	−723.846	13.038
3000	82.395	444.717	374.453	210.794	−950.366	−716.047	12.467
3100	82.442	447.420	376.763	219.036	−951.062	−708.225	11.934
3200	82.484	450.038	379.012	227.282	−951.735	−700.381	11.433
3300	82.523	452.577	381.203	235.533	−952.382	−692.516	10.962
3400	82.559	455.041	383.339	243.787	−953.002	−684.632	10.518
3500	82.591	457.434	385.422	252.044	−953.594	−676.730	10.100
3600	82.621	459.762	387.455	260.305	−954.157	−668.811	9.704
3700	82.649	462.026	389.440	268.569	−954.688	−660.878	9.330
3800	82.674	464.230	391.379	276.835	−955.187	−652.931	8.975
3900	82.698	466.378	393.275	285.103	−955.652	−644.970	8.638
4000	82.720	468.472	395.128	293.374	−956.083	−636.998	8.318
4100	82.740	470.515	396.942	301.647	−956.479	−629.016	8.014
4200	82.759	472.509	398.718	309.922	−1436.688	−614.001	7.636
4300	82.776	474.456	400.457	318.199	−1435.923	−594.422	7.221
4400	82.793	476.360	402.160	326.477	−1435.123	−574.861	6.824
4500	82.808	478.220	403.830	334.757	−1434.286	−555.319	6.446
4600	82.822	480.041	405.467	343.039	−1433.413	−535.796	6.084
4700	82.836	481.822	407.073	351.322	−1432.504	−516.292	5.738
4800	82.848	483.566	408.648	359.606	−1431.558	−496.808	5.406
4900	82.860	485.274	410.194	367.891	−1430.576	−477.345	5.089
5000	82.871	486.948	411.713	376.178	−1429.558	−457.901	4.784
5100	82.882	488.590	413.204	384.466	−1428.504	−438.479	4.491
5200	82.892	490.199	414.669	392.754	−1427.415	−419.077	4.210
5300	82.901	491.778	416.109	401.044	−1426.291	−399.696	3.939
5400	82.910	493.328	417.525	409.335	−1425.133	−380.337	3.679
5500	82.919	494.849	418.917	417.626	−1423.941	−361.000	3.428
5600	82.926	496.343	420.287	425.918	−1422.716	−341.685	3.187
5700	82.934	497.811	421.634	434.211	−1421.459	−322.392	2.954
5800	82.941	499.254	422.960	442.505	−1420.171	−303.122	2.730
5900	82.948	500.672	424.265	450.800	−1418.852	−283.873	2.513
6000	82.954	502.066	425.550	459.095	−1417.504	−264.648	2.304

PREVIOUS: December 1964 (1 atm) CURRENT· December 1964 (1 bar)

Chlorodifluoroborane (BClF$_2$) B$_1$Cl$_1$F$_2$(g)

Boron Chloride Oxide (OBCl) IDEAL GAS $M_r = 62.2624$ Boron Chloride Oxide (OBCl) $B_1Cl_1O_1(g)$

$S°(298.15\ K) = [237.42]\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = [-316.8 \pm 29]\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = -316.3 \pm 29\ kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm $^{-1}$
[690](1)
[400](2)
[1850](1)

Ground State Quantum Weight: [1] $\sigma = 1$
Point Group: [$C_{\infty v}$]
Bond Distances: Cl–B = [1.75] Å; B–O = [1.20] Å
Bond Angle: Cl–B–O = [180]°
Rotational Constant: $B_0 = [0.165056]\ cm^{-1}$

Enthalpy of Formation

The vapor–phase equilibria existing in the $B_2O_3 + BCl_3$ system were determined by an effusion method in the temperature range 1234–1389 K by Blauer and Farber.[1] Based on the equilibrium constants reported for the reaction 1/3 $B_2O_3(l)$ + 1/3 $BCl_3(g)$ = BOCl(g), the 2nd and 3rd law values of $\Delta_r H°(298.15\ K)$ were evaluated as *57.7 and 56.3 kcal·mol^{-1}*, respectively. The 3rd law value for $\Delta_r H°(298.15\ K)$ was adopted for the calculation of the enthalpy of formation, $\Delta_f H°$(BOCl, g, 298.15 K).

Heat Capacity and Entropy

The molecular structure is assumed to be linear. The vibrational frequencies are estimated from the values calculated by the valence force method described by Herzberg[2] using estimated force constants, $k_1 = 5.2 \times 10^5$, $k_2 = 16.7 \times 10^5$ dynes·cm^{-1} and $k_3 = 0.40 \times 10^{-11}$ dynes·cm·rad^{-1}. The B=O and B–Cl bond distances were assumed to be the same as those in BO(g) and $BCl_3(g)$, respectively.

References

[1] J. Blauer and M. Farber, Trans. Faraday Soc. 60, 301 (1964).
[2] G. Herzberg, Infrared and Raman Spectra, D. van Nostrand Company, Inc., (1945).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.609	−316.774	−316.774	INFINITE
100	30.896	196.590	273.283	−7.669	−316.766	−318.278	166.252
200	39.254	220.565	241.372	−4.161	−316.565	−319.850	83.536
250	42.577	229.698	238.145	−2.112	−316.425	−320.687	67.004
298.15	45.040	237.417	237.417	0.	−316.310	−321.519	56.329
300	45.123	237.696	237.418	0.083	−316.307	−321.551	55.987
350	47.105	244.806	237.975	2.391	−316.224	−322.432	48.120
400	48.708	251.204	239.235	4.788	−316.185	−323.323	42.222
450	50.054	257.021	240.893	7.258	−316.190	−324.215	37.634
500	51.216	262.356	242.776	9.790	−316.229	−325.105	33.963
600	53.146	271.871	246.852	15.012	−316.384	−326.867	28.456
700	54.680	280.184	251.032	20.406	−316.608	−328.597	24.520
800	55.909	287.568	255.146	25.938	−316.878	−330.291	21.566
900	56.898	294.213	259.124	31.580	−317.180	−331.950	19.266
1000	57.696	300.250	262.939	37.311	−317.511	−333.574	17.424
1100	58.344	305.781	266.586	43.114	−317.867	−335.163	15.916
1200	58.875	310.881	270.068	48.976	−318.250	−336.719	14.657
1300	59.313	315.611	273.391	54.886	−318.659	−338.242	13.591
1400	59.677	320.020	276.566	60.836	−319.096	−339.732	12.676
1500	59.982	324.148	279.602	66.819	−319.563	−341.190	11.881
1600	60.239	328.028	282.509	72.831	−320.062	−342.615	11.185
1700	60.459	331.687	285.295	78.866	−320.593	−344.009	10.570
1800	60.647	335.148	287.969	84.921	−321.159	−345.370	10.022
1900	60.809	338.431	290.540	90.994	−321.760	−346.699	9.531
2000	60.949	341.554	293.013	97.083	−322.400	−347.995	9.089
2100	61.072	344.531	295.396	103.184	−323.078	−349.258	8.687
2200	61.180	347.374	297.694	109.296	−323.797	−350.488	8.322
2300	61.275	350.096	299.914	115.419	−324.557	−351.685	7.987
2400	61.359	352.706	302.060	121.551	−375.620	−351.778	7.656
2500	61.434	355.212	304.136	127.691	−376.545	−350.766	7.329
2600	61.500	357.623	306.147	133.837	−377.482	−349.716	7.026
2700	61.560	359.945	308.097	139.991	−378.433	−348.630	6.745
2800	61.614	362.185	309.989	146.149	−379.397	−347.509	6.483
2900	61.663	364.348	311.826	152.313	−380.376	−346.353	6.238
3000	61.707	366.439	313.612	158.482	−381.370	−345.163	6.010
3100	61.747	368.463	315.349	164.655	−382.379	−343.939	5.795
3200	61.784	370.424	317.039	170.831	−383.402	−342.683	5.594
3300	61.817	372.326	318.686	177.011	−384.440	−341.395	5.404
3400	61.848	374.172	320.291	183.194	−385.491	−340.074	5.225
3500	61.876	375.965	321.856	189.381	−386.554	−338.723	5.055
3600	61.902	377.708	323.384	195.570	−387.629	−337.341	4.895
3700	61.925	379.405	324.875	201.761	−388.715	−335.930	4.742
3800	61.947	381.057	326.332	207.955	−389.810	−334.488	4.598
3900	61.968	382.666	327.756	214.150	−390.913	−333.018	4.460
4000	61.987	384.235	329.148	220.348	−392.023	−331.519	4.329
4100	62.004	385.766	330.510	226.548	−393.138	−329.993	4.204
4200	62.021	387.260	331.844	232.749	−874.106	−321.415	3.997
4300	62.036	388.720	333.150	238.952	−874.141	−308.255	3.745
4400	62.050	390.146	334.429	245.156	−874.179	−295.095	3.503
4500	62.064	391.541	335.683	251.362	−874.219	−281.934	3.273
4600	62.076	392.905	336.912	257.569	−874.261	−268.771	3.052
4700	62.088	394.240	338.117	263.777	−874.303	−255.608	2.841
4800	62.099	395.547	339.300	269.986	−874.346	−242.444	2.638
4900	62.109	396.828	340.461	276.197	−874.388	−229.278	2.444
5000	62.119	398.083	341.601	282.408	−874.429	−216.113	2.258
5100	62.128	399.313	342.721	288.620	−874.470	−202.946	2.079
5200	62.137	400.519	343.821	294.834	−874.509	−189.779	1.906
5300	62.145	401.703	344.902	301.048	−874.547	−176.610	1.741
5400	62.153	402.865	345.964	307.263	−874.585	−163.441	1.581
5500	62.160	404.005	347.009	313.478	−874.621	−150.272	1.427
5600	62.167	405.125	348.037	319.695	−874.657	−137.101	1.279
5700	62.174	406.226	349.048	325.912	−874.694	−123.930	1.136
5800	62.180	407.307	350.044	332.129	−874.731	−110.758	0.997
5900	62.186	408.370	351.023	338.348	−874.769	−97.587	0.864
6000	62.191	409.415	351.988	344.566	−874.809	−84.414	0.735

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

Boron Chloride Oxide (OBCl) $B_1Cl_1O_1(g)$

Dichloroborane (BCl_2) IDEAL GAS $M_r = 81.716$ Dichloroborane (BCl_2) $B_1Cl_2(g)$

$\Delta_f H°(0\ K) = -80.9 \pm 17.6\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = [272.7 \pm 2.1]\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = -79.5 \pm 12.6\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights	
ϵ_i, cm^{-1}	g_i
0	2
[11000]	[2]
28003	1
28153	1
29455	1
29542	1

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[700] (1)
250 (1)
[725] (1)

Point Group: $[C_{2v}]$ $\sigma = 2$

Bond Distance: B–Cl = [1.73] Å

Bond Angle: Cl–B–Cl = [112]°

Product of the Moments of Inertia: $I_A I_B I_C = 9.065976 \times 10^{-115}\ g^3 \cdot cm^6$

Enthalpy of Formation

Srivastava and Farber[1] have investigated the equilibrium vapors over the boron trichloride–boron system by mass spectrometry. Gaseous BCl_3 was allowed to flow into a boron nitride effusion cell which contained metallic boron. A flow variation study indicated that thermal equilibrium had been achieved during their experiments. Ion intensities for the species $BCl_3(g)$, $BCl_2(g)$, and $BCl(g)$ were measured at electron energies slightly above appearance potentials in the temperature range 1513 to 1813 K. JANAF analysis of equiibrium constants for the reaction $BCl_3(g) + BCl(g) = 2BCl_2(g)$ which are obtained from their ion intenesity data yields a 3rd law $\Delta_r H$(298.15 K) value of 24.56 ± 1.00 $kcal \cdot mol^{-1}$ with a drift of −2.1 ± 2.0 $cal \cdot K^{-1} mol^{-1}$. The 2nd law $\Delta_r H$ value at 298.15 K is 28.1 $kcal \cdot mol^{-1}$. Using the 3rd law $\Delta_r H$ value in conjunction with JANAF enthalpies of formation[2] for $BCl_3(g)$ and $BCl(g)$ and $BCl(g)$, we calculate $\Delta_f H°(BCl_2$, g, 298.15 K) = −19.0 ± 3.0 $kcal \cdot mol^{-1}$.

The only other reported data on the enthalpy of formation of BCl_2 comes from explosion studies carried out at elevated temperatures by Rusin and Tatevskii.[3] The BCl_2 radical was found to be stable at 2250 K in H_2–Cl_2–BCl_3 mixtures. These workers reported $\Delta_f H°(BCl_2$, g, 298.15 K) = −18.4 ± 1.5 $kcal \cdot mol^{-1}$ which confirms the results of Srivastava and Farber.[1]

We adopt $\Delta_f H°(BCl_2$, g, 298.15 K) = −19.0 ± 3.0 $kcal \cdot mol^{-1}$. This value also leads to a realistic progression in the stepwise bond dissociation energies for BCl(g), $BCl_2(g)$, and $BCl_3(g)$. Using all JANAF data,[2] we calculate D_1(B–Cl) = 127.9, D_2(BCl–Cl) = 81.7, and $D_3(BCl_2$–Cl) = 106.2 $kcal \cdot mol^{-1}$. This bond energy scheme, $D_1 > D_2 < D_3$, is consistent with that predicted for the Group III A fluorides by Hildenbrand.[4]

Heat Capacity and Entropy

The point group and the Cl–B–Cl bond angle are assumed to be the same as those for BF_2.[2] The B–Cl bond length is estimated to lie between those for BCl and BCl_3.[2] The principal moments of inertia are: $I_A = 1.4577 \times 10^{-39}$, $I_B = 24.2203 \times 10^{-39}$, and $I_C = 25.6780 \times 10^{-39}\ g \cdot cm^2$.

Dessaux *et al.*[5,6] observed a diffuse system of bands in the near ultraviolet which they attributed to the BCl_2 radical. The emission spectrum was obtained as chemiluminescence in the reaction between BCl_3 and atomic hydrogen. They indicated that the frequencies $\nu_1 = 470$, $\nu_2 = 240$, and $\nu_3 = 990\ cm^{-1}$ were consistent with their spectral data, however, alternate assignments are possible. We prefer the frequencies $\nu_1 = 700$, ν_2 250, and $\nu_3 = 725\ cm^{-1}$, since these values are more consistent with those for CCl_2, $SiCl_2$, and $AlCl_2$.[2]

By analogy with the isoelectronic molecule NO_2,[7] the ground state for BCl_2 is assumed to be $^2A_1$. Huckel-molecular-orbital calculations by Hastie and Margrave[8] suggest a doublet excited state ($^2B_1$) near 11,000 cm^{-1} which is included. The upper electronic levels are those observed by Dessaux *et al.*[6]

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0	INFINITE	−11.759	−80.860	−80.860	INFINITE
100	36.437	227.742	311.228	−8.349	−80.386	−84.228	43.996
200	42.282	254.796	276.857	−4.412	−79.820	−88.303	23.062
250	45.066	264.535	273.444	−2.227	−79.625	−90.447	18.898
298.15	47.375	272.677	272.677	0.	−79.496	−92.544	16.213
300	47.455	272.970	272.678	0.088	−79.492	−92.625	16.127
350	49.389	280.436	273.263	2.511	−79.415	−94.821	14.151
400	50.918	287.135	274.585	5.020	−79.392	−97.024	12.670
450	52.122	293.205	276.322	7.597	−79.419	−99.226	11.518
500	53.073	298.747	278.292	10.228	−79.487	−101.424	10.596
600	54.439	308.553	282.540	15.608	−79.720	−105.792	9.210
700	55.341	317.018	286.874	21.100	−80.055	−110.112	8.217
800	55.962	324.450	291.116	26.667	−80.470	−114.378	7.468
900	56.404	331.069	295.194	32.287	−80.953	−118.588	6.883
1000	56.729	337.029	299.085	37.944	−81.494	−122.741	6.411
1100	56.975	342.448	302.784	43.630	−82.088	−126.838	6.023
1200	57.166	347.414	306.299	49.337	−82.732	−130.878	5.697
1300	57.319	351.996	309.641	55.062	−83.421	−134.862	5.419
1400	57.445	356.248	312.820	60.800	−84.154	−138.792	5.178
1500	57.553	360.215	315.849	66.550	−84.930	−142.668	4.968
1600	57.650	363.933	318.739	72.310	−85.745	−146.491	4.782
1700	57.740	367.431	321.501	78.080	−86.601	−150.262	4.617
1800	57.828	370.733	324.146	83.858	−87.494	−153.981	4.468
1900	57.917	373.862	326.681	89.646	−88.426	−157.649	4.334
2000	58.009	376.836	329.115	95.442	−89.395	−161.268	4.212
2100	58.106	379.668	331.455	101.248	−90.400	−164.837	4.100
2200	58.207	382.374	333.708	107.063	−91.442	−168.357	3.997
2300	58.315	384.963	335.881	112.889	−92.521	−171.829	3.902
2400	58.428	387.448	337.978	118.726	−143.896	−174.185	3.791
2500	58.547	389.835	340.005	124.575	−145.127	−175.422	3.665
2600	58.671	392.134	341.966	130.436	−146.363	−176.609	3.548
2700	58.800	394.350	343.865	136.309	−147.605	−177.748	3.439
2800	58.932	396.491	345.707	142.196	−148.852	−178.842	3.336
2900	59.067	398.562	347.494	148.096	−150.105	−179.891	3.240
3000	59.205	400.566	349.230	154.010	−151.365	−180.897	3.150
3100	59.344	402.510	350.917	159.937	−152.629	−181.860	3.064
3200	59.484	404.396	352.559	165.878	−153.899	−182.783	2.984
3300	59.623	406.229	354.158	171.834	−155.172	−183.666	2.907
3400	59.762	408.011	355.716	177.803	−156.448	−184.510	2.835
3500	59.900	409.745	357.235	183.786	−157.726	−185.317	2.766
3600	60.037	411.435	358.717	189.783	−159.003	−186.087	2.700
3700	60.171	413.081	360.164	195.793	−160.278	−186.822	2.637
3800	60.302	414.688	361.578	201.817	−161.548	−187.523	2.578
3900	60.431	416.256	362.960	207.854	−162.812	−188.190	2.521
4000	60.557	417.787	364.312	213.903	−164.066	−188.824	2.466
4100	60.680	419.284	365.634	219.965	−165.310	−189.428	2.413
4200	60.800	420.748	366.929	226.039	−646.390	−182.977	2.276
4300	60.917	422.180	368.197	232.125	−646.518	−171.942	2.089
4400	61.030	423.582	369.440	238.223	−646.629	−160.904	1.910
4500	61.140	424.954	370.659	244.331	−646.723	−149.864	1.740
4600	61.247	426.299	371.854	250.451	−646.796	−138.821	1.576
4700	61.351	427.618	373.026	256.581	−646.848	−127.778	1.420
4800	61.452	428.910	374.177	262.721	−646.878	−116.733	1.270
4900	61.550	430.179	375.307	268.871	−646.882	−105.689	1.127
5000	61.645	431.423	376.417	275.031	−646.862	−94.644	0.989
5100	61.737	432.645	377.507	281.200	−646.814	−83.600	0.856
5200	61.827	433.844	378.579	287.378	−646.739	−72.558	0.729
5300	61.914	435.023	379.633	293.565	−646.635	−61.517	0.606
5400	61.999	436.181	380.670	299.761	−646.503	−50.478	0.488
5500	62.081	437.319	381.689	305.965	−646.341	−39.441	0.375
5600	62.161	438.439	382.693	312.177	−646.149	−28.409	0.265
5700	62.239	439.540	383.680	318.397	−645.927	−17.380	0.159
5800	62.316	440.623	384.653	324.625	−645.675	−6.354	0.057
5900	62.390	441.689	385.611	330.860	−645.393	4.666	−0.041
6000	62.462	442.738	386.554	337.102	−645.082	15.681	−0.137

PREVIOUS: June 1972 (1 atm) CURRENT: June 1972 (1 bar)

Dichloroborane, Ion (BCl_2^+) IDEAL GAS $M_r = 81.71545$ Dichloroborane, Ion (BCl_2^+) $B_1Cl_2^+(g)$

$S°(298.15\ K) = [257.8 \pm 8.4]\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = 665.4 \pm 25\ kJ\cdot mol^{-1}$

$\Delta_f H°(298.15\ K) = 674.0 \pm 25\ kJ\cdot mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^1\Sigma_g^+$	0	1
$^1B_2$	[16000]	1
$^1A_1$	[35000]	1

Vibrational Frequencies and Degeneracies

ν, cm^{-1}
[500] (1)
[150] (2)
[800] (1)

Point Group: $[D_{\infty h}]$ σ = 2

Bond Distances. B–Cl = [1.74] Å

Bond Angle: Cl–B–Cl = [180]°

Product of the Moments of Inertia: $B_0 = [0.078526]\ cm^{-1}$

Enthalpy of Formation

The appearance potential of the positive ion fragment $BCl_2^+(g)$ from $BCl_3(g)$ was determined mass spectrometrically by Osberghaus,[1] Marriott,[2] and Koski[3] as 13.2 ± 0.5, 13.01 ± 0.02, and 11.8 ± 0.2 eV, respectively. From the reaction $BCl_3 + e^- = BCl_2^+ + Cl + 2e^-$, the corresponding values of $\Delta_f H°(298.15\ K)$ for $BCl_2^+(g)$ are derived to be 181.9 ± 11.5, 177.5 ± 0.5, and 149.6 ± 4.6 kcal·mol^{-1}, using $\Delta_f H°(0\ K) = -96.078$ and 28.520 kcal·mol^{-1} for $BCl_3(g)$ and Cl(g). These electron impact values are superseded by the photoionization results of Dibeler and Walker[7] who report the onset of BCl_2^+ from BCl_3 as 12.30 ± 0.02 eV (283.65 ± 0.05 kcal·mol^{-1}). This yields $\Delta_f H°(0\ K) = 159.05 \pm 0.6$ kcal·mol^{-1} or $\Delta_f H°(298.15\ K) = 161.1 \pm 0.6$ kcal·mol^{-1}, which are adopted.

Heat Capacity and Entropy

The molecular structure is assumed to be linear using the Walsh[4] predictions for 16 valence electron XY_2 molecules. The electronic states, levels and vibrational frequencies are estimated by comparison with those for CO_2.[5] The B–Cl bond distance is estimated using the method of Krasnov.[6]

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	-12.848	665.391		
100	40.874	206.815	301.467	-9.465			
200	48.200	237.603	262.511	-4.982			
250	50.884	248.657	258.666	-2.502			
298.15	52.974	257.805	257.805	0.	674.042	659.173	-115.484
300	53.046	258.133	257.806	0.098	674.095	659.081	-114.756
350	54.747	266.443	258.459	2.795	675.485	656 468	-97.972
400	56.076	273.844	259.928	5.567	676.810	653.660	-85.359
450	57 115	280.511	261.851	8.397	678.076	650.690	-75.530
500	57.934	286.573	264.024	11.274	679.294	647.581	-67.652
600	59.110	297.247	268.696	17.131	681.616	641.018	-55.806
700	59.887	306.422	273.445	23.083	683.820	634.076	-47.315
800	60.422	314.455	278.080	29.100	685.933	626.825	-40.927
900	60.803	321.595	282.526	35.163	687.972	619.313	-35.944
1000	61.084	328.017	286.759	41.258	689.946	611.578	-31.946
1100	61.296	333.849	290.779	47.377	691.864	603.648	-28.665
1200	61.460	339.190	294.594	53.515	693.730	595.546	-25.923
1300	61.588	344.115	298.216	59.668	695.548	587.290	-23.598
1400	61.692	348.683	301.660	65.832	697.319	578.895	-21.599
1500	61.776	352.942	304.938	72.006	699.046	570.376	-19.862
1600	61.846	356.931	308.064	78.187	700.730	561.743	-18.339
1700	61.904	360.682	311.050	84.374	702.371	553.006	-16.992
1800	61.955	364.222	313.907	90.567	703.970	544.173	-15.791
1900	61.999	367.573	316.644	96.765	705.528	535.253	-14.715
2000	62.038	370.754	319.271	102.967	707.044	526.252	-13.744
2100	62.075	373.782	321.795	109.173	708.517	517.176	-12.864
2200	62.110	376.671	324.224	115.382	709.947	508.030	-12.062
2300	62.145	379.432	326.565	121.595	711.333	498.821	-11.329
2400	62.180	382.078	328.823	127.811	662.416	490.621	-10.678
2500	62.216	384.617	331.005	134.031	663.634	483.438	-10.101
2600	62.254	387.058	333.114	140.254	664.840	476.207	-9.567
2700	62.295	389.408	335.156	146.482	666.031	468.929	-9.072
2800	62.339	391.674	337.134	152.713	667.207	461.607	-8.611
2900	62.387	393.863	339.053	158.949	668.369	454.244	-8.182
3000	62.437	395.979	340.915	165.191	669.516	446.841	-7.780
3100	62.492	398.027	342.724	171.437	670.649	439.399	-7.404
3200	62.551	400.012	344.484	177.689	671.768	431.922	-7.050
3300	62.613	401.937	346.196	183.947	672.876	424.410	-6.718
3400	62.679	403.808	347.863	190.212	673.974	416.864	-6.404
3500	62.749	405.625	349.487	196.483	675.063	409.286	-6.108
3600	62.822	407.394	351.071	202.762	676.147	401.677	-5.828
3700	62.899	409.117	352.617	209.048	677.226	394.038	-5.563
3800	62.978	410.795	354.126	215.342	678.305	386.369	-5.311
3900	63.061	412.432	355.600	221.644	679.385	378.673	-5.072
4000	63.145	414.030	357.041	227.954	680.469	370.949	-4.844
4100	63.232	415.590	358.450	234.273	681.561	363.197	-4.627
4200	63.321	417.115	359.829	240.601	202.814	362.443	-4.508
4300	63.412	418.606	361.178	246.937	205.015	366.218	-4.449
4400	63.504	420.065	362.500	253.283	207.231	369.941	-4.392
4500	63.597	421.493	363.795	259.638	209.462	373.614	-4.337
4600	63.690	422.891	365.065	266.002	211.712	377.237	-4.284
4700	63.785	424.262	366.310	272.376	213.982	380.811	-4.232
4800	63.879	425.606	367.531	278.759	216.275	384.336	-4.182
4900	63.974	426.924	368.730	285.152	218.591	387.814	-4.134
5000	64.069	428.218	369.907	291.554	220.933	391.243	-4.087
5100	64.163	429.487	371.063	297.966	223.302	394.626	-4.042
5200	64.257	430.734	372.198	304.387	225.699	397.962	-3.998
5300	64.351	431.959	373.314	310.817	228.124	401.251	-3.955
5400	64.443	433.163	374.411	317.257	230.579	404.495	-3.913
5500	64.535	434.346	375.490	323.706	233.065	407.693	-3.872
5600	64.626	435.510	376.552	330.164	235.581	410.845	-3.832
5700	64.715	436.654	377.596	336.631	238.129	413.953	-3.793
5800	64.804	437.781	378.624	343.107	240.707	417.015	-3.756
5900	64.891	438.889	379.636	349.592	243.317	420.032	-3.719
6000	64.977	439.981	380.633	356.085	245.958	423.005	-3.683

PREVIOUS: December 1970 (1 atm) CURRENT. December 1970 (1 bar)

Dichloroborane, Ion (BCl_2^+) $B_1Cl_2^+(g)$

Dichloroborane, Ion (BCl_2^-) IDEAL GAS $M_r = 81.71655$ Dichloroborane, Ion (BCl_2^-) $B_1Cl_2^-(g)$

$\Delta_fH°(0\ K) = [-142 \pm 105]\ kJ\cdot mol^{-1}$

$S°(298.15\ K) = [266.3 \pm 4.2]\ J\cdot K^{-1}\cdot mol^{-1}$ $\Delta_fH°(298.15\ K) = [-146 \pm 105]\ kJ\cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^1A_1$	0	1
$^3B_1$	[12000]	3
$^1B_1$	[17000]	1

Vibrational Frequencies and Degeneracies
ν, cm^{-1}
[750] (1)
[250] (1)
[775] (1)

Point Group: [C_{2v}] $\sigma = 2$

Bond Distances: B–Cl = [1.716] Å

Bond Angle: Cl–B–Cl = [100]°

Product of the Moments of Inertia: $I_AI_BI_C = [8.575781 \times 10^{-115}]\ g^3\cdot cm^6$

Enthalpy of Formation

The enthalpy of formation $\Delta_fH°(BCl_2^-, g, 0\ K) = -33.8 \pm 25\ kcal\cdot mol^{-1}$, is obtained from an estimated electron affinity for BCl_2 and $\Delta_fH°(BCl_2, g, 0\ K) = -19.3 \pm 3.0\ kcal\cdot mol^{-1}$.[1] Comparison of the ionization potentials and electron affinities for the isoelectronic molecules NO_2,[1,2] BF_2,[1] and AlF_2[1] indicates that in each case the difference between these two quantities (IP–EA) is roughly 7.1 eV. From this relationship, we estimate EA (BCl_2) = 0.63 ± 1.0 eV with IP (BCl_2) = 7.73 eV.[1]

Heat Capacity and Entropy

The correlation diagram of Walsh[3] predicts a bent configuration for BCl_2^- (18 valence electrons) with a bond angle considerably reduced from that for BCl_2. Based on the adopted angle for BCl_2 (112°),[1] we estimate the angle in BCl_2^- at 100°. Comparison with angles for CF_2 and SiF_2[1] indicates that the estimated angle is reasonable. The B–Cl bond length is taken equal to that for BCl.[1] The principal moments of inertia are: $I_A = 1.8951 \times 10^{-39}$, $I_B = 20.3463 \times 10^{-39}$, and $I_C = 22.2413 \times 10^{-39}\ g\cdot cm^2$.

The ground state electronic configuration ($^1A_1$) and first excited singlet state ($^1B_1$) for BCl_2^- are estimated by analogy with those for CCl_2 and $SiCl_2$.[1] Also included is a triplet level at 12000 cm^{-1}. The energy separation (5000 cm^{-1}) of the $^3B_1$ and $^1B_1$ levels is estimated by comparison with the corresponding values for SO_2,[4] $SiCl_2$,[1] $GeCl_2$, and $SnCl_2$.[5] The vibrational frequencies are estimated from those for BCl_2, CCl_2, and $SiCl_2$.[1]

References

[1] JANAF Thermochemical Tables: $BCl_2(g)$, $NO_2^-(g)$, $BF_2^-(g)$, $AlF_2^-(g)$, 6–30–72, $BF_2^+(g)$, $BCl_2^+(g)$, and $SiCl_2(g)$, 12–31–70; $CF_2(g)$, 6–30–70; $SiF_2(g)$ and $CCl_2(g)$, 12–31–68; BCl(g), 12–31–64.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−11.666	−141.514		
100	36.409	221.745	304.298	−8.255			
200	41.747	248.642	270.365	−4.345			
250	44.356	258.240	267.006	−2.191			
298.15	46.614	266.251	266.251	0.	−146.440	−151.317	26.510
300	46.694	266.539	266.252	0.086	−146.476	−151.348	26.352
350	48.651	273.889	266.828	2.472	−147.476	−152.081	22.697
400	50.236	280.493	268.130	4.945	−148.528	−152.668	19.936
450	51.507	286.486	269.842	7.490	−149.627	−153.120	17.774
500	52.524	291.968	271.784	10.092	−150.763	−153.447	16.031
600	54.006	301.684	275.979	15.423	−153.123	−153.764	13.386
700	54.997	310.089	280.265	20.877	−155.575	−153.679	11.468
800	55.684	317.480	284.464	26.413	−158.100	−153.236	10.005
900	56.176	324.068	288.505	32.007	−160.687	−152.473	8.849
1000	56.540	330.007	292.363	37.643	−163.328	−151.420	7.909
1100	56.815	335.409	296.035	43.312	−166.018	−150.099	7.128
1200	57.030	340.362	299.525	49.005	−168.754	−148.531	6.465
1300	57.203	344.934	302.845	54.716	−171.535	−146.734	5.896
1400	57.346	349.179	306.004	60.444	−174.357	−144.720	5.400
1500	57.472	353.140	309.016	66.185	−177.220	−142.504	4.962
1600	57.590	356.853	311.891	71.938	−180.122	−140.095	4.574
1700	57.705	360.347	314.640	77.703	−183.060	−137.503	4.225
1800	57.826	363.649	317.272	83.480	−186.035	−134.738	3.910
1900	57.958	366.779	319.796	89.269	−189.043	−131.806	3.624
2000	58.105	369.756	322.220	95.072	−192.083	−128.715	3.362
2100	58.270	372.594	324.552	100.890	−195.155	−125.471	3.121
2200	58.456	375.309	326.797	106.726	−198.255	−122.080	2.899
2300	58.664	377.912	328.964	112.582	−201.383	−118.548	2.692
2400	58.896	380.414	331.056	118.460	−254.796	−113.810	2.477
2500	59.151	382.823	333.078	124.362	−258.052	−107.869	2.254
2600	59.428	385.149	335.037	130.291	−261.299	−101.797	2.045
2700	59.727	387.397	336.935	136.248	−264.535	−95.601	1.850
2800	60.044	389.575	338.776	142.237	−267.759	−89.285	1.666
2900	60.379	391.688	340.564	148.258	−270.970	−82.855	1.492
3000	60.728	393.740	342.303	154.313	−274.166	−76.313	1.329
3100	61.090	395.737	343.994	160.404	−277.346	−69.666	1.174
3200	61.460	397.683	345.642	166.531	−280.508	−62.916	1.027
3300	61.837	399.580	347.248	172.696	−283.650	−56.068	0.887
3400	62.218	401.432	348.814	178.899	−286.772	−49.124	0.755
3500	62.600	403.241	350.343	185.140	−289.870	−42.090	0.628
3600	62.980	405.009	351.837	191.419	−292.943	−34.967	0.507
3700	63.355	406.740	353.298	197.736	−295.990	−27.759	0.392
3800	63.725	408.435	354.727	204.090	−299.009	−20.469	0.281
3900	64.086	410.095	356.125	210.480	−301.997	−13.100	0.175
4000	64.436	411.722	357.495	216.907	−304.954	−5.654	0.074
4100	64.775	413.317	358.837	223.367	−307.878	1.865	−0.024
4200	65.100	414.882	360.153	229.861	−790.616	16.478	−0.205
4300	65.411	416.417	361.443	236.387	−792.383	35.716	−0.434
4400	65.706	417.924	362.710	242.943	−794.114	54.994	−0.653
4500	65.984	419.404	363.954	249.527	−795.810	74.311	−0.863
4600	66.246	420.857	365.175	256.139	−797.470	93.666	−1.064
4700	66.490	422.285	366.375	262.776	−799.094	113.055	−1.256
4800	66.716	423.687	367.554	269.437	−800.681	132.480	−1.442
4900	66.924	425.065	368.714	276.119	−802.233	151.937	−1.620
5000	67.114	426.419	369.855	282.821	−803.748	171.425	−1.791
5100	67.287	427.749	370.977	289.541	−805.228	190.943	−1.956
5200	67.442	429.058	372.081	296.277	−806.673	210.490	−2.114
5300	67.580	430.344	373.168	303.029	−808.084	230.064	−2.267
5400	67.701	431.608	374.239	309.793	−809.461	249.665	−2.415
5500	67.806	432.851	375.293	316.568	−810.806	269.291	−2.558
5600	67.896	434.074	376.332	323.354	−812.120	288.941	−2.695
5700	67.970	435.276	377.356	330.147	−813.404	308.614	−2.828
5800	68.030	436.459	378.364	336.947	−814.658	328.310	−2.957
5900	68.076	437.622	379.359	343.753	−815.885	348.027	−3.081
6000	68.109	438.767	380.340	350.562	−817.085	367.764	−3.202

PREVIOUS: June 1972 (1 atm) CURRENT: June 1972 (1 bar)

Dichloroborane, Ion (BCl_2^-) $B_1Cl_2^-(g)$

Dichlorofluoroborane (BCl_2F) IDEAL GAS $M_r = 100.714403$ Dichlorofluoroborane (BCl_2F) $B_1Cl_2F_1(g)$

$S°(298.15\ K) = 287.7\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -643 \pm 21\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -644 \pm 21\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}
1320 (1)	1000 (1)
[554] (1)	[339] (1)
[266] (1)	528 (1)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: B–Cl = [1.73] Å; B–F = [1.295] Å
Bond Angles: Cl–B–Cl = [120]°; F–B–Cl = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = 1.202356 \times 10^{-113}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The values for BCl_2F and $BClF_2$ of $\Delta_fH°(298.15\ K) = -154$ and $\Delta_fH°(298.15\ K) = -211.6\ kcal{\cdot}mol^{-1}$, respectively, are obtained from the average bond energies of BF_3 and BCl_3. The calculated values were each made less negative by about 0.8 $kcal{\cdot}mol^{-1}$ in order to make them consistent with the equilibrium measurements of Higgins, Leisegang, Raw, and Rossouw,[1] and Gunn and Sanborn[2] for the reaction.

$$BF_3(g) + BCl_3(g) \rightarrow BClF_2(g) + BCl_2F(g).$$

Values for the enthalpy of reaction are $\Delta_rH(298.15\ K) = +1.68\ kcal{\cdot}mol^{-1}$ and $\Delta_rH(298.15\ K) = 1\ 1$ (uncertainty of -0.5 to $+0.8$) $kcal{\cdot}mol^{-1}$, the former calculated from the measured equilibrium constant and the statistical entropy change and the latter obtained from the variation of the equilibrium constant with temperature. Selection of $\Delta_rH(298.15\ K) = 1.6\ kcal{\cdot}mol^{-1}$ fixes the sum of the enthalpies of formation of $BClF_2$ and BCl_2F as *−365.6 kcal·mol⁻¹, but it does not determine the individual values*. Thus, the selected enthalpies of formation are only as accurate as the average bond energy calculations on which they are based. A reasonable estimate of the uncertainty would be ±5 $kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

The spectroscopic constants are based on the work of Lindeman and Wilson,[3] who observed ν_1, ν_4, and ν_6 and calculated ν_2, ν_3, and ν_5. The frequencies were adjusted to the normal isotopic composition of 81.2% ^{11}B and 18.8% ^{10}B. The bond angles were taken to be 120° while the bond lengths were assumed to be the same as in the respective trihalides. The principal moments of inertia are $I_A = 11.8761 \times 10^{-39}$, $I_B = 26.4297 \times 10^{-39}$, and $I_C = 38.3059 \times 10^{-39}\ g{\cdot}cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−13.267	−642.796	−642.796	INFINITE
100	37.983	235.579	333.920	−9.834	−643.752	−639.860	334.229
200	50.361	265.837	292.820	−5.397	−644.150	−635.776	166.048
250	55.201	277.612	288.627	−2.754	−644.248	−633.670	132.398
298.15	59.063	287.675	287.675	0.	−644.336	−631.625	110.658
300	59.198	288.041	287.677	0.109	−644.339	−631.546	109.962
350	62.535	297.425	288.410	3.155	−644.434	−629.407	93.934
400	65.335	305.963	290.078	6.354	−644.537	−627.253	81.911
450	67.688	313.799	292.285	9.681	−644.647	−625.086	72.558
500	69.666	321.036	294.803	13.117	−644.759	−622.906	65.075
600	72.738	334.024	300.282	20.245	−644.981	−618.515	53.847
700	74.942	345.412	305.933	27.635	−645.194	−614.087	45.824
800	76.552	355.529	311.512	35.214	−645.402	−609.629	39.805
900	77.751	364.618	316.916	42.932	−645.613	−605.145	35.122
1000	78.662	372.860	322.105	50.755	−645.834	−600.636	31.374
1100	79.368	380.391	327.066	58.658	−646.071	−596.105	28.307
1200	79.923	387.322	331.803	66.623	−646.330	−591.552	25.750
1300	80.367	393.737	336.323	74.638	−646.613	−586.975	23.585
1400	80.726	399.707	340.640	82.694	−646.924	−582.377	21.729
1500	81.022	405.287	344.766	90.782	−647.267	−577.754	20.119
1600	81.267	410.524	348.714	98.896	−647.643	−573.108	18.710
1700	81.472	415.457	352.496	107.034	−648.053	−568.437	17.466
1800	81.646	420.119	356.125	115.190	−648.499	−563.741	16.359
1900	81.795	424.537	359.610	123.362	−648.981	−559.020	15.369
2000	81.922	428.736	362.962	131.548	−649.501	−554.271	14.476
2100	82.033	432.736	366.190	139.746	−650.057	−549.496	13.668
2200	82.129	436.554	369.302	147.954	−650.652	−544 694	12.933
2300	82.213	440.207	372.306	156.171	−651.284	−539.864	12.261
2400	82.288	443.708	375.209	164.396	−702.212	−533.936	11.621
2500	82.353	447.068	378.017	172.629	−702.997	−526.909	11.009
2600	82.412	450.299	380.735	180.867	−703.787	−519.850	10.444
2700	82.464	453.410	383.369	189.111	−704.581	−512.760	9.920
2800	82.511	456.410	385.925	197.360	−705.380	−505.641	9.433
2900	82.554	459.307	388.406	205.613	−706.183	−498.493	8.979
3000	82.592	462.106	390.816	213.870	−706.989	−491.318	8.555
3100	82.626	464.815	393.159	222.131	−707.798	−484.115	8.157
3200	82.658	467.438	395.440	230.395	−708.607	−476.887	7.784
3300	82.687	469.982	397.660	238.663	−709.417	−469.633	7.434
3400	82.713	472.451	399.824	246.933	−710.225	−462.355	7.103
3500	82.737	474.849	401.933	255.205	−711.029	−455.053	6.791
3600	82.759	477.180	403.991	263.480	−711.827	−447.728	6.496
3700	82.779	479.448	406.000	271.757	−712.617	−440.381	6.217
3800	82.798	481.656	407.962	280.036	−713.398	−433.013	5.952
3900	82.815	483.807	409.880	288.316	−714.166	−425.624	5.701
4000	82.832	485.904	411.754	296.599	−714.919	−418.216	5.461
4100	82.846	487.949	413.588	304.883	−715.655	−410.789	5.234
4200	82.860	489.946	415.382	313.168	−1196.221	−396.321	4.929
4300	82.873	491.896	417.139	321.455	−1195.828	−377.280	4.583
4400	82.885	493.801	418.860	329.743	−1195.413	−358.249	4.253
4500	82.897	495.664	420.546	338.032	−1194.975	−339.227	3.938
4600	82.907	497.486	422.199	346.322	−1194.510	−320.216	3.636
4700	82.917	499.269	423.820	354.613	−1194.018	−301.215	3.348
4800	82.927	501.015	425.410	362.905	−1193.497	−282.224	3.071
4900	82.935	502.725	426.970	371.198	−1192.946	−263.245	2.806
5000	82.944	504.401	428.502	379.492	−1192.364	−244.278	2.552
5100	82.951	506.043	430.006	387.787	−1191.750	−225.322	2.308
5200	82.959	507.654	431.484	396.083	−1191.103	−206.378	2.073
5300	82.965	509.234	432.936	404.379	−1190.423	−187.448	1.847
5400	82.972	510.785	434.364	412.676	−1189.709	−168.530	1.630
5500	82.978	512.308	435.767	420.973	−1188.961	−149.626	1.421
5600	82.984	513.803	437.147	429.271	−1188.178	−130.736	1.219
5700	82.990	515.272	438.505	437.570	−1187.361	−111.861	1.025
5800	82.995	516.715	439.841	445.869	−1186.510	−93.000	0.838
5900	83.000	518.134	441.156	454.169	−1185.625	−74.153	0.657
6000	83.005	519.529	442.451	462.469	−1184.707	−55.323	0.482

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Dichloroborane (BHCl$_2$) IDEAL GAS $M_r = 82.72394$ Dichloroborane (BHCl$_2$) B$_1$Cl$_2$H$_1$(g)

$S°(298.15\ \mathrm{K}) = [268.3]\ \mathrm{J{\cdot}K^{-1}{\cdot}mol^{-1}}$

$\Delta_f H°(0\ \mathrm{K}) = -245 \pm 4\ \mathrm{kJ{\cdot}mol^{-1}}$
$\Delta_f H°(298.15\ \mathrm{K}) = -248 \pm 4\ \mathrm{kJ{\cdot}mol^{-1}}$

Vibrational Frequencies and Degeneracies υ, cm⁻¹	υ, cm⁻¹
[2610] (1)	1091 (1)
744 (1)	[894] (1)
[287] (1)	786 (1)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: B–H = 1.13 ± 0.2 Å; B–Cl = [1.75] Å
Bond Angles: Cl–B–Cl = 119.7 ± 3°; Cl–B–H = 120.15 ± 1.5°
Product of the Moments of Inertia: $I_A I_B I_C = 1.392331 \times 10^{-114}\ \mathrm{g^3{\cdot}cm^6}$

Enthalpy of Formation

The chemical equilibria for the following two reactions: (A) $BCl_3(g) + H_2(g) = BHCl_2(g) + HCl(g)$, and (B) $6BHCl_2(g) = B_2H_6(g) + 4BCl_3(l, g)$ were investigated by Murib, Horvitz, and Bonecutter,[1] Mook, Seiler, and Watson[2] and Lynds and Bass.[3] Using the reported equilibrium constants, the corresponding enthalpy changes and the respective $\Delta_f H°(298.15\ \mathrm{K})$ values were evaluated. The results obtained are presented as follows.

Source	Reaction	T/K	$\Delta_r H°$(298.15 K), kcal·mol⁻¹ 2nd law	3rd law	$\Delta_f H°$(298.15 K) kcal·mol⁻¹
[1]	A	873 – 973	15.57 ± 0.8	16.19	−58.06 ± 0.5
[2]	A	1073 – 1273	13.50 ± 3.0	13.91	−60.3 ± 0.7
[1]	B	273	—	−17.85	−59.6
[3]	B	298	—	−19.09	−59.4

The value of $\Delta_f H°(298.15\ \mathrm{K})$ for $BHCl_2(g)$ is selected as − 59.3 ± 1 kcal·mol⁻¹.

Heat Capacity and Entropy

The molecular structure, B–H bond distance and Cl–B–Cl bond angle were obtained from Lynds and Bass.[4] The B–Cl bond distance was assumed to be the same as that in $BCl_3(g)$. The vibrational frequencies adopted were reported by Bass, Lynds, Wolfram, DeWames[5] and corrected to the average isotopic species. It has been pointed out that the complete assignment of the infrared spectra of $HBCl_2(g)$ is quite difficult due to the unavoidable presence of $BCl_3(g)$. The adopted frequencies were obtained using the Green's function and partitioning techniques, taking $HBCl_2$ as an "isotopic" species of BCl_3. An excellent agreement between the calculated and observed spectra reported Lynds and Bass[5] was claimed. Spectra of the mixture of BCl_3, $HBCl_2$ and $DBCl_2$ are quite complex and have been observed by Lynds and Stern,[6] Nadean and Oaks,[7] Mayers and Putnam[8] and only three bands were correlated with $HBCl_2$. Analysis of infrared data from previous works, according to the conventional Wilson's method of symmetry coordinates, has been undertaken by de Mandirola and Westerkamp.[9] Based on four observed frequencies, a set of six frequencies was derived and assigned. The principal moments of inertia are: $I_A = 1.7957 \times 10^{-39}$, $I_B = 26.9625 \times 10^{-39}$, and $I_C = 28.7581 \times 10^{-39}\ \mathrm{g{\cdot}cm^2}$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.744	−245.227	−245.227	INFINITE
100	35.653	223.535	307.156	−8.362	−246.280	−244.666	127.800
200	41.988	250.084	272.565	−4.496	−247.132	−242.731	63.395
250	45.882	259.867	269.069	−2.301	−247.624	−241.574	50.474
298.15	49.644	268.272	268.272	0.	−248.111	−240.365	42.111
300	49.784	268.580	268.273	0.092	−248.130	−240.317	41.843
350	53.357	276.528	268.893	2.672	−248.620	−238.976	35.665
400	56.480	283.862	270.311	5.420	−249.087	−237.566	31.023
450	59.157	290.673	272.200	8.313	−249.528	−236.099	27.406
500	61.447	297.027	274.369	11.329	−249.941	−234.584	24.507
600	65.120	308.571	279.127	17.666	−250.682	−231.442	20.149
700	67.933	318.829	284.080	24.325	−251.320	−228.183	17.027
800	70.157	328.051	289.009	31.233	−251.870	−224.839	14.680
900	71.956	336.422	293.820	38.342	−252.351	−221.431	12.852
1000	73.433	344.082	298.468	45.614	−252.780	−217.972	11.386
1100	74 657	351.140	302.940	53.020	−253.173	−214.472	10.184
1200	75.681	357.682	307.233	60.539	−253.544	−210.937	9.182
1300	76.543	363.774	311.350	68.151	−253.906	−207.372	8.332
1400	77.274	369.474	315.301	75.843	−254.268	−203.779	7.603
1500	77.896	374.827	319.092	83.602	−254.638	−200.160	6.970
1600	78.430	379.872	322.735	91.419	−255.022	−196.515	6.416
1700	78.890	384.641	326.238	99.286	−255.427	−192.846	5.925
1800	79.289	389.162	329.609	107.195	−255.857	−189.153	5.489
1900	79.636	393.458	332.857	115.142	−256.316	−185.435	5.098
2000	79.941	397.551	335.990	123.121	−256.806	−181.692	4.745
2100	80.208	401.458	339.016	131.129	−257.332	−177.923	4.426
2200	80.445	405.195	341.939	139.162	−257.897	−174.129	4.134
2300	80.654	408.775	344.768	147.217	−258.502	−170.308	3.868
2400	80.841	412.212	347.507	155.292	−309.410	−165.391	3.600
2500	81.009	415.516	350.162	163.384	−310.182	−159.374	3.330
2600	81.159	418.696	352.737	171.493	−310.969	−153.326	3.080
2700	81.294	421.761	355.237	179.616	−311.774	−147.248	2.849
2800	81.416	424.720	357.666	187.751	−312.597	−141.139	2.633
2900	81.526	427.579	360.028	195.898	−313.440	−135.001	2.432
3000	81.627	430.345	362.326	204.056	−314.303	−128.833	2.243
3100	81.718	433.023	364.563	212.223	−315.188	−122.636	2.066
3200	81.802	435.618	366.744	220.399	−316.094	−116.411	1.900
3300	81.878	438.137	368.869	228.584	−317.021	−110.156	1.744
3400	81.949	440.582	370.942	236.775	−317.967	−103.874	1.596
3500	82.013	442.959	372.966	244.973	−318.932	−97.563	1.456
3600	82.073	445.270	374.943	253.177	−319.914	−91.224	1.324
3700	82.128	447.519	376.874	261.388	−320.911	−84.858	1.198
3800	82.179	449.710	378.762	269.603	−321.921	−78.464	1.079
3900	82.226	451.845	380.609	277.823	−322.943	−72.044	0.965
4000	82.270	453.928	382.416	286.048	−323.974	−65.598	0.857
4100	82.311	455.960	384.185	294.277	−325.011	−59.126	0.753
4200	82.349	457.944	385.917	302.510	−805.902	−45.604	0.567
4300	82.385	459.882	387.615	310.747	−805.857	−27.502	0.334
4400	82.418	461.776	389.279	318.987	−805.813	−9.401	0.112
4500	82.449	463.629	390.911	327.231	−805.769	8.698	−0.101
4600	82.478	465.441	392.511	335.477	−805.720	26.797	−0.304
4700	82.506	467.215	394.082	343.726	−805.667	44.895	−0.499
4800	82.532	468.953	395.624	351.978	−805.606	62.991	−0.685
4900	82.556	470.655	397.138	360.232	−805.537	81.086	−0.864
5000	82.579	472.323	398.625	368.489	−805.456	99.180	−1.036
5100	82.600	473.958	400.086	376.748	−805.364	117.272	−1.201
5200	82.621	475.562	401.522	385.009	−805.258	135.361	−1.360
5300	82.640	477.136	402.934	393.272	−805.138	153.449	−1.512
5400	82.658	478.681	404.322	401.537	−805.002	171.535	−1.659
5500	82.675	480.198	405.688	409.804	−804.849	189.617	−1.801
5600	82.691	481.688	407.032	418.072	−804.679	207.697	−1.937
5700	82.707	483.152	408.355	426.342	−804.491	225.773	−2.069
5800	82.722	484.590	409.657	434.613	−804.283	243.847	−2.196
5900	82.736	486.004	410.939	442.886	−804.056	261.916	−2.319
6000	82.749	487.395	412.202	451.161	−803.809	279.981	−2.437

PREVIOUS: March 1966 (1 atm) CURRENT: March 1966 (1 bar)

Trichloroborane (BCl$_3$) IDEAL GAS M_r = 117.169 Trichloroborane (BCl$_3$) B$_1$Cl$_3$(g)

$\Delta_f H°(0\ K) = -402.0 \pm 2.1\ kJ\cdot mol^{-1}$

$S°(298.15\ K) = 290.17\ J\cdot K^{-1}\cdot mol^{-1}$ $\Delta_f H°(298.15\ K) = -403.0 \pm 2.1\ kJ\cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}
471.0 (1)	986.3 (2)
470.6 (1)	243.0 (1)

Ground State Quantum Weight: 1 $\sigma = 6$

Point Group: D_{3h}

Bond Distance: B−Cl = 1.75 Å

Bond Angle: Cl−B−Cl = 120°

Product of the Moments of Inertia: $I_A I_B I_C = 3.956022 \times 10^{-113}\ g^3\cdot cm^6$

Enthalpy of Formation

The enthalpy change of the reaction B(am) + 3/2 Cl$_2$(g) = BCl$_3$(g) has been determined in a calorimeter by Johnson, Miller and Prosen.[1] From the reported value $\Delta_r H°(298.15\ K) = -97.51 + 0.32\ kcal\cdot mol^{-1}$, the enthalpy of formation for BCl$_3$(g) was derived as $-96.31 \pm 0.50\ kcal\cdot mol^{-1}$, using $\Delta_r H°(298.15\ K) = 1.20 \pm 0.40\ kcal\cdot mol^{-1}$ for the reaction B(cr) = B(am). Some other related enthalpies of reaction reported by previous investigators are presented as follows.

Source	Reaction	$\Delta_r H°(298.15\ K)$ kcal·mol^{-1}	$\Delta_f H°(298.15\ K)$ kcal·mol^{-1}
[2]	B(am) + 3/2 Cl$_2$(g) = BCl$_3$(g)	−97.4 ± 0.7	−96.2 ± 0.8
	B(am) + 3/2 Cl$_2$(g) = BCl$_3$(l)	−103.3 ± 0.6	−96.5 ± 0.7
[3]	B$_2$H$_6$(g) + 6 Cl$_2$(g) = 2 BCl$_3$(g) + 6 HCl(g)	−342.9	−100.4 ± 5.0
[4]	BCl$_3$(l) + (n+3)H$_2$O(l) = (H$_3$BO$_3$+3HCl)n H$_2$O (Sln)	−69.2 ± 1.0	−97.2 ± 1.0
[5]	BCl$_3$(l) + 2403 H$_2$O(l) = (H$_3$BO$_3$+3HCl)2400 H$_2$O (Sln)	−68.68 ± 0.06	−96.3 ± 0.2
[6]	BCl$_3$(l) + 593 H$_2$O(l) = (H$_3$BO$_3$+3HCl)590 H$_2$O (Sln)	−69.12 ± 0.11	−95.44 ± 0.39

The enthalpies of formation for BCl$_3$(l) derived from the enthalpies of hydrolysis reported by other investigatoars were reviewed by Johnson, Miller and Prosen.[1]

Heat Capacity and Entropy

The bond distance of B and Cl atoms has been reported to be 1.73 ± 0.02 and 1.76 ± 0.02, 1.75 Å by Levy and Brockway,[7] Gregg, Hampson and Jenkins, Jones, and Sutton,[8] and Spencer and Lipscomb,[9] respectively. The last value is adopted. The values of vibrational frequencies used were reported by Lindeman and Wilson.[10] The vibrational frequencies were also determined by Cassie,[11] Lassettre and Yost,[12] Scruby, Lacher and Park.[13] The molecular structure was given by Levy amd Brockway.[7] The principal moments of inertia are: $I_A = I_B = 27.0443 \times 10^{-39}$, and $I_C = 54.0887 \times 10^{-39}\ g\cdot cm^2$.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−14.021	−401.997	−401.997	INFINITE
100	40.687	234.433	339.441	−10.501	−402.868	−397.930	207.857
200	53.832	266.971	295.623	−5.730	−402.987	−392.909	102.617
250	58.598	279.513	291.176	−2.916	−402.972	−390.391	81.568
298.15	62.392	290.169	290.169	0.	−402.961	−387.969	67.971
300	62.524	290.555	290.170	0.116	−402.961	−387.876	67.535
350	65.763	300.445	290.944	3.325	−402.956	−385.362	57.512
400	68.421	309.406	292.700	6.682	−402.962	−382.849	49.995
450	70.595	317.594	295.018	10.159	−402.976	−380.334	44.148
500	72.374	325.127	297.657	13.735	−402.997	−377.817	39.470
600	75.037	338.574	303.383	21.114	−403.047	−372.776	32.453
700	76.872	350.287	309.265	28.715	−403.109	−367.726	27.440
800	78.172	360.641	315.053	36.471	−403.185	−362.667	23.680
900	79.118	369.906	320.642	44.338	−403.281	−357.596	20.754
1000	79.824	378.280	325.994	52.286	−403.399	−352.514	18.413
1100	80.363	385.915	331.099	60.297	−403.544	−347.419	16.498
1200	80.783	392.926	335.963	68.355	−403.717	−342.309	14.900
1300	81.116	399.406	340.597	76.451	−403.922	−337.184	13.548
1400	81.384	405.427	345.016	84.576	−404.159	−332.041	12.389
1500	81.603	411.050	349.233	92.726	−404.430	−326.881	11.383
1600	81.783	416.322	353.263	100.895	−404.736	−321.701	10.502
1700	81.934	421.285	357.119	109.081	−405.079	−316.501	9.725
1800	82.062	425.972	360.816	117.281	−405.460	−311.280	9.033
1900	82.170	430.412	364.363	125.493	−405.881	−306.036	8.414
2000	82.263	434.629	367.771	133.715	−406.343	−300.770	7.855
2100	82.344	438.645	371.052	141.945	−406.848	−295.479	7.350
2200	82.414	442.477	374.212	150.183	−407.398	−290.163	6.889
2300	82.475	446.142	377.260	158.428	−407.995	−284.821	6.468
2400	82.529	449.653	380.204	166.678	−458.902	−278.383	6.059
2500	82.576	453.023	383.050	174.933	−459.679	−270.845	5.659
2600	82.619	456.262	385.804	183.193	−460.477	−263.276	5.289
2700	82.656	459.381	388.471	191.457	−461.298	−255.676	4.946
2800	82.690	462.388	391.058	199.724	−462.144	−248.045	4.627
2900	82.721	465.290	393.568	207.995	−463.016	−240.383	4.330
3000	82.748	468.095	396.005	216.268	−463.914	−232.691	4.052
3100	82.773	470.809	398.375	224.544	−464.839	−224.968	3.791
3200	82.796	473.437	400.680	232.823	−465.789	−217.216	3.546
3300	82.816	475.985	402.923	241.104	−466.764	−209.432	3.315
3400	82.835	478.458	405.109	249.386	−467.762	−201.620	3.098
3500	82.853	480.859	407.239	257.671	−468.781	−193.777	2.892
3600	82.868	483.193	409.317	265.957	−469.818	−185.905	2.697
3700	82.883	485.464	411.344	274.244	−470.871	−178.004	2.513
3800	82.896	487.675	413.324	282.533	−471.935	−170.075	2.338
3900	82.909	489.828	415.258	290.823	−473.008	−162.117	2.171
4000	82.921	491.927	417.149	299.115	−474.086	−154.132	2.013
4100	82.931	493.975	418.997	307.408	−475.164	−146.120	1.862
4200	82.941	495.973	420.807	315.701	−956.089	−131.057	1.630
4300	82.950	497.925	422.577	323.996	−956.071	−111.414	1.353
4400	82.959	499.832	424.312	332.291	−956.044	−91.771	1.089
4500	82.967	501.697	426.011	340.588	−956.005	−72.129	0.837
4600	82.975	503.520	427.676	348.885	−955.950	−52.487	0.596
4700	82.982	505.305	429.309	357.182	−955.878	−32.848	0.365
4800	82.989	507.052	430.910	365.481	−955.783	−13.210	0.144
4900	82.995	508.763	432.482	373.780	−955.665	6.426	−0.069
5000	83.001	510.440	434.024	382.080	−955.521	26.059	−0.272
5100	83.006	512.084	435.539	390.380	−955.348	45.689	−0.468
5200	83.012	513.696	437.026	398.681	−955.145	65.315	−0.656
5300	83.016	515.277	438.488	406.983	−954.909	84.937	−0.837
5400	83.021	516.829	439.924	415.284	−954.641	104.554	−1.011
5500	83.026	518.352	441.336	423.587	−954.337	124.167	−1.179
5600	83.030	519.848	442.725	431.890	−953.998	143.773	−1.341
5700	83.034	521.318	444.091	440.193	−953.623	163.372	−1.497
5800	83.037	522.762	445.435	448.496	−953.210	182.966	−1.648
5900	83.041	524.181	446.758	456.800	−952.760	202.551	−1.793
6000	83.044	525.577	448.060	465.105	−952.273	222.128	−1.934

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Fluoroborane (BF) IDEAL GAS $M_r = 29.808403$

$S°(298\ 15\ \text{K}) = 200.479\ \text{J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0\ \text{K}) = -119.0 \pm 13.8\ \text{kJ·mol}^{-1}$
$\Delta_f H°(298.15\ \text{K}) = -115.9 \pm 13.8\ \text{kJ·mol}^{-1}$

Electronic Level and Quantum Weight State	ϵ_i, cm^{-1}	g_i
$^1\Sigma^+$	0	1

$\omega_e = 1410.3\ \text{cm}^{-1}$ $\omega_e x_e = 11.98\ \text{cm}^{-1}$ $\sigma = 1$
$B_e = 1.5286\ \text{cm}^{-1}$ $\alpha_e = 0.0168\ \text{cm}^{-1}$ $r_e = 1.265$ Å

Enthalpy of Formation

The equilibria of the reaction 2/3 B(cr) + 1/3 $BF_3(g) = BF(g)$ were studied by Blauer, Greenbaum and Farber[1] by means of transpiratio at pressures below 300 µ. The values of log $K_p°$ at 1375 and 1476 K were reported as −3.99 ± 0.02 and −3.30 ± 0.05, respectively. By the 3rd law method the value of $\Delta_r H°$(298 15 K) for the reaction was derived to be 61 38 kcal·mol^{-1}, yielding $\Delta_f H°$(BF, g, 298.15 K) = −28.7 ± 2.6 kcal·mol^{-1}. The system B + CaF_2 was studied mass spectrometrically in a graphite Knudsen cell by Hildenbrand.[6] The equilibria involving BF(g) were observed. Intensity measurements were made at temperatures, 1583 1734 K. From the 3rd law value, $\Delta_r H°$(298.15 K) = 12.2 + 0.3 kcal·mol^{-1}, for the reaction $BF_3(g) + Ca(g) = BF(g) + CaF_2(g)$, the value of $\Delta_f H$d(298.15 K) for BF(g) was derived as −26.7 ± 2 kcal·mol^{-1}. The dissociation energy of BF(g) molecule has been reported by Herzberg,[2] Gaydon[3] and Barrow.[4] The corresponding values of $\Delta_f H°$(298.15 K) for BF(g) were derived. The results are compared with those obtained from equilibrium data as follows:

Source	Reaction	$\Delta_r H°$(298.15 K) kcal·mol^{-1}	$\Delta_f H°$(298.15 K) kcal·mol^{-1}
1	2/3 B(cr) + 1/3 $BF_3(g) = BF(g)$	61.38	−28.7 ± 2.6
2	$BF(g) = B(g) + F(g)$	100.2	+51.5
3	$BF(g) = B(g) + F(g)$	197.0	−45.3 ± 11.5
4	$BF(g) = B(g) + F(g)$	186.0	−34.3
5	2/3 B(cr) + 1/3 $BF_3 = BF(g)$	—	−28 ± 3
6	$BF_3(g) + Ca(g) = BF(g) + CaF_2(g)$	12.2	−26.7 ± 2

The value of $\Delta_f H°$(298.15 K) adopted is the average of the first and last $\Delta_f H°$(298.15 K) values listed in the above table.

Heat Capacity and Entropy

The spectroscopic constants used were obtained from Onaka[7] and to the average isotopic species. Spectroscopic constants for BF(g) were also reported by Herzberg.[2]

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Fluoroborane (BF) $B_1F_1(g)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8 694	−118.965	−118.965	INFINITE
100	29.108	168.594	226.494	−5.790	−117.538	−125.848	65 736
200	29.154	188.777	203.167	−2.878	−116.423	−134 630	35.162
250	29.302	195.296	200.965	−1.417	−116.085	−139.224	29.089
298.15	29.591	200.479	200.479	0.	−115.897	−143.699	25.176
300	29.605	200.662	200.480	0.055	−115.892	−143.872	25.050
350	30.047	205.258	200.842	1.546	−115.823	−148.542	22.169
400	30.579	209.304	201.652	3.061	−115.858	−153.215	20.008
450	31.149	212.939	202.707	4.604	−115.976	−157.879	18.326
500	31.719	216.250	203.898	6.176	−116.157	−162.525	16.979
600	32.768	222.128	206.459	9.401	−116.649	−171.755	14.953
700	33.646	227.247	209.071	12.724	−117.258	−180.893	13.498
800	34.356	231.788	211.632	16.125	−117 944	−189.937	12.402
900	34.926	235.869	214.102	19.590	−118.688	−198.892	11.543
1000	35.385	239.573	216.467	23.107	−119 479	−207.762	10.852
1100	35.757	242.964	218.724	26.664	−120.311	−216.550	10.283
1200	36 064	246 089	220.876	30.256	−121.181	−225.261	9.805
1300	36.319	248.986	222.928	33.875	−122.088	−233.898	9.398
1400	36.535	251.686	224.887	37.518	−123 030	−242.464	9.046
1500	36.719	254.213	226.759	41.181	−124.006	−250.961	8.739
1600	36.879	256.588	228.549	44.861	−125.017	−259.392	8.468
1700	37.018	258.828	230.265	48.556	−126.061	−267.758	8.227
1800	37 141	260.947	231 911	52.264	−127.137	−276 062	8.011
1900	37.252	262.958	233.493	55.984	−128.245	−284.306	7.816
2000	37.351	264.872	235.014	59.714	−129.383	−292.490	7.639
2100	37.441	266.696	236.480	63.454	−130.549	−300.617	7.477
2200	37.524	268.440	237.893	67.202	−131.743	−308.688	7.329
2300	37.601	270.110	239.258	70.959	−132.961	−316.704	7.193
2400	37.672	271.712	240.577	74.722	−184.463	−323.597	7.043
2500	37.739	273.251	241.854	78.493	−185.804	−329.367	6.882
2600	37.801	274.732	243.090	82.270	−187.134	−335.083	6.732
2700	37.861	276.160	244.288	86.053	−188.449	−340.748	6.592
2800	37.917	277.538	245.451	89.842	−189.749	−346.365	6.462
2900	37.971	278.869	246.581	93.636	−191.032	−351.936	6.339
3000	38.023	280.157	247.679	97.436	−192.298	−357.463	6.224
3100	38.072	281.405	248.747	101.241	−193.545	−362.948	6.116
3200	38.120	282.615	249.786	105.051	−194.774	−368.393	6.013
3300	38.167	283.788	250.799	108.865	−195.982	−373.799	5.917
3400	38.212	284.928	251.786	112.684	−197.170	−379.170	5.825
3500	38.256	286.037	252.749	116.507	−198.338	−384.506	5.738
3600	38.299	287.115	253.689	120.335	−199.484	−389.808	5.656
3700	38.341	288.165	254.606	124 167	−200.610	−395.080	5.578
3800	38.382	289.188	255.503	128.003	−201.714	−400.321	5.503
3900	38.422	290.185	256.379	131.843	−202.797	−405.533	5.432
4000	38.461	291.159	257.237	135.687	−203.859	−410.718	5.363
4100	38.500	292.109	258.076	139.536	−204.900	−415.877	5.298
4200	38.539	293.037	258.897	143.388	−685.770	−413.986	5.149
4300	38.576	293.944	259.702	147.243	−685.683	−407.516	4.950
4400	38 614	294.832	260.490	151.103	−685.577	−401.048	4.761
4500	38.651	295.700	261.263	154.966	−685.454	−394.583	4.580
4600	38.687	296.550	262.021	158.833	−685.313	−388.120	4.407
4700	38.723	297.382	262.764	162.703	−685.156	−381.661	4.242
4800	38.759	298.198	263.494	166.578	−684.984	−375.206	4.083
4900	38.794	298.997	264.210	170.455	−684.796	−368.754	3.931
5000	38.830	299 781	264 914	174.336	−684.594	−362.306	3.785
5100	38.865	300.551	265.605	178.221	−684.378	−355.863	3.645
5200	38.899	301.306	266.285	182.109	−684.149	−349.423	3.510
5300	38.934	302.047	266.952	186.001	−683.908	−342.989	3.380
5400	38.968	302 775	267.609	189.896	−683.656	−336.558	3.256
5500	39 002	303.490	268.255	193.795	−683.393	−330.133	3.135
5600	39 036	304.193	268.890	197.696	−683.120	−323.713	3.019
5700	39.069	304.885	269.516	201.602	−682.837	−317.297	2.908
5800	39.103	305.564	270.132	205.510	−682.547	−310.887	2.800
5900	39.136	306.233	270.738	209.422	−682.248	−304.481	2.696
6000	39.169	306.891	271.335	213.338	−681.943	−298.081	2.595

PREVIOUS: December 1964 (1 atm) CURRENT. December 1964 (1 bar)

Fluoroborane (BF) $B_1F_1(g)$

$S°(298.15\ K) = [224.8]\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = -602 \pm 13\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -602 \pm 13\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm $^{-1}$
[1050](1)
[500](2)
[1900](1)

Ground State Quantum Weight: [1] $\sigma = 1$
Point Group: $[C_{\infty v}]$
Bond Distances: B–F = [1.30] Å; B–O = [1.20] Å
Bond Angle: O–B–F = [180]°
Rotational Constant: $B_0 = [0.309392]\ cm^{-1}$

Enthalpy of Formation

The equilbrium constants for the reaction $B_2O_3(l) + BF_3(g) = 3\ BOF(g)$ in the temperature range 1054–1253 K were determined by Farber and Blauer[1] using the so-called Molecular Flow Reaction Method. The value of $\Delta_r H°$ for this reaction was evaluated by both the 2nd and 3rd law methods, using the equilibrium constants corrected for the trimer and correcting $K_p°$ at 1200 K from 9.6×10^{-11} to 9.6×10^{-10}. Hildebrand, Theard and Saul[2] analyzed the vapor above mixture of MgF_2 and B_2O_3 contained in a Knudsen cell with a mass spectrometer and found that in the temperature range 980–1230 K the vapor is composed of $BF_3(g)$, $(BOF)_3(g)$ and BOF(g) species. From the reported temperature dependence of appropriate ion intensities the enthalpy change of the reaction $(BOF)_3(g) = 3\ BOF(g)$ was derived by the 2nd law method as 127.9 $kcal \cdot mol^{-1}$ at 1115 K or 129.75 $kcal \cdot mol^{-1}$ at 298.15 K. The results obtained are presented as follows, using JANAF free energy functions and auxiliary data.

Source	Reaction	$\Delta_r H°(298.15\ K)$, $kcal \cdot mol^{-1}$ $kcal \cdot mol^{-1}$		$\Delta_f H°(298.15\ K)$ $kcal \cdot mol^{-1}$
Farber and Blauer	$B_2O_3(l) + BF_3(g) = 3\ BOF(g)$	150.2 ± 16.6	149.0	−140.1 ± 6*
Hildenbrand *et al.*	$(BOF)_3(g) = 3\ BOF(g)$	129.8 ± 3	–	−145.2 ± 1.5

*Calculation based on the 3rd law value and one point rejected due to statistical test.

The adopted value of $\Delta_f H°(298.15\ K)$ for BOF(g) is the weighted average of the two values listed above.

Heat Capacity and Entropy

The molecular structure is assumed to be linear. The vibrational frequencies (ν) are estimated from the values calculated by the valence force method described by Herzberg[3] using estimated force constants, $k_1 = 10 \times 10^5$ dynes cm^{-1} and $k_2 = 0.47 \times 10^{-11}$ dynes cm rad^{-1}. The B=O and B–F bond distances are assumed to be the same as those in BO(g) and $BF_3(g)$ molecules.

References

[1] M. Farber and J. Blauer, Trans. Faraday Soc. 58, 2090 (1962)
[2] D. L. Hildenbrand, L. P. Theard, and A. M. Saul, J. Chem. Phys. 39, 1973 (1963).
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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.934	−602.462	−602.462	INFINITE
100	29.748	187.280	257.440	−7.016	−602.474	−603.987	315 491
200	35.585	209.533	228.390	−3 771	−602.482	−605.491	158 138
250	38.542	217.799	225.465	−1.916	−602.478	−606.244	126.668
298.15	40.996	224.803	224.803	0.	−602.496	−606.969	106.338
300	41.083	225.057	224.804	0.076	−602.497	−606.996	105.687
350	43.261	231.558	225.312	2.186	−602.547	−607.743	90.701
400	45.151	237.461	226.468	4.397	−602.634	−608.479	79.459
450	46.811	242.877	227.994	6.697	−602.754	−609.203	70.714
500	48.281	247.886	229.736	9.075	−602.899	−609.912	63.717
600	50.752	256.916	233.530	14.032	−603.240	−611.284	53.217
700	52.719	264.893	237.452	19.209	−603.621	−612.594	45.712
800	54.286	272.039	241.336	24.562	−604.024	−613.849	40.080
900	55.539	278.508	245.113	30.056	−604.442	−615.052	35.697
1000	56.547	284.413	248.752	35.662	−604.874	−616.208	32.187
1100	57.362	289.842	252.244	41.359	−605.322	−617.320	29.314
1200	58.028	294.863	255.589	47.129	−605.787	−618.390	26.918
1300	58.575	299.530	258.792	52.960	−606.274	−619.421	24.889
1400	59.030	303.888	261.859	58.841	−606.785	−620.413	23.148
1500	59.410	307.974	264.798	64.764	−607.323	−621.368	21.638
1600	59.731	311.819	267.618	70.721	−607.889	−622.286	20.316
1700	60.004	315.449	270.326	76.708	−608.487	−623.168	19.148
1800	60.238	318.885	272.929	82.721	−609.117	−624 014	18.108
1900	60.439	322.147	275.434	88.755	−609.780	−624.823	17.178
2000	60.614	325.252	277.848	94.808	−610.477	−625.597	16.339
2100	60.766	328.213	280.177	100.877	−611.206	−626.335	15.579
2200	60.900	331.043	282.425	106.960	−611.969	−627 038	14 888
2300	61.017	333 753	284.598	113.056	−612.763	−627.705	14.256
2400	61 121	336.352	286.701	119.163	−663.847	−627.269	13.652
2500	61.214	338.849	288.737	125.280	−664.780	−625.725	13.074
2600	61.297	341.252	290.711	131.406	−665.709	−624.145	12.539
2700	61.371	343.566	292.626	137.539	−666.632	−622.528	12.044
2800	61.438	345.800	294 485	143.680	−667.549	−620.878	11.583
2900	61 498	347.957	296.292	149.827	−668.459	−619.196	11.153
3000	61.553	350.042	298.049	155.979	−669.361	−617.481	10.751
3100	61.603	352.061	299.759	162.137	−670.253	−615.737	10.375
3200	61.648	354.018	301.424	168.300	−671.135	−613.965	10.022
3300	61.689	355.916	303.047	174.466	−672.007	−612.165	9.690
3400	61.727	357.758	304.629	180.637	−672.867	−610.338	9.377
3500	61.762	359.548	306.173	186.812	−673.715	−608.487	9.081
3600	61.794	361.288	307.680	192.989	−674.552	−606.611	8.802
3700	61.823	362.981	309.152	199.170	−675.375	−604.713	8.537
3800	61.850	364.631	310.590	205.354	−676.186	−602.792	8.286
3900	61.876	366.237	311.996	211.540	−676.984	−600.850	8.047
4000	61.899	367.804	313.372	217.729	−677.769	−598.888	7.821
4100	61 921	369.333	314 718	223.920	−678.542	−596.906	7.605
4200	61.941	370.825	316 037	230.113	−1159.151	−587.882	7.311
4300	61.960	372.283	317.328	236.308	−1158.811	−574.284	6.976
4400	61.978	373.708	318.593	242.505	−1158.461	−560.694	6.656
4500	61.994	375.101	319.833	248.704	−1158.101	−547.113	6.351
4600	62.009	376.464	321.050	254.904	−1157.733	−533.540	6.059
4700	62.024	377.797	322.243	261.106	−1157.356	−519.974	5.779
4800	62.038	379.103	323.414	267.309	−1156.972	−506.417	5.511
4900	62.050	380.383	324.564	273.513	−1156.581	−492.867	5.254
5000	62.062	381.636	325.693	279.719	−1156.185	−479.326	5.007
5100	62.074	382.865	326.802	285.925	−1155.784	−465.793	4.771
5200	62.084	384.071	327.891	292.133	−1155.380	−452.268	4.543
5300	62.095	385.254	328.963	298.342	−1154 973	−438.750	4.324
5400	62.104	386.414	330.016	304.552	−1154.565	−425.241	4.113
5500	62.113	387.554	331.052	310.763	−1154.157	−411.739	3.910
5600	62.122	388.673	332.071	316.975	−1153.750	−398.243	3.715
5700	62.130	389.773	333.073	323.188	−1153.345	−384.756	3.526
5800	62 138	390.853	334.060	329.401	−1152.943	−371.275	3.344
5900	62.145	391.916	335.032	335.615	−1152.546	−357.802	3.168
6000	62 152	392.960	335.989	341.830	−1152.155	−344.335	2.998

PREVIOUS December 1965 (1 atm) CURRENT December 1965 (1 bar)

Difluoroborane (BF_2) IDEAL GAS $M_r = 48.806806$ Difluoroborane (BF_2) $B_1F_2(g)$

$S°(298.15\ K) = [247.16 \pm 2.1]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -590.5 \pm 13\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = -589.9 \pm 13\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^2A_1$	0	2
$^2B_1$	[16000]	2

Vibrational Frequencies and Degeneracies

ν, cm^{-1}
[1080](1)
[500](1)
[1213](1)

Point Group: C_{2v} $\sigma = 2$

Bond Distance: B–F = [1.30] Å

Bond Angle: F–B–F = 112°

Product of Moments of Inertia: $I_A I_B I_C = [4.36647 \times 10^{-116}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

Srivastava and Farber,[1] using a gas inlet boron nitride effusion cell, performed a mass spectrometric study of the equilibrium vapor species over the system $BF_3(g) + B(cr)$. Ion intensities for $BF_3(g)$, $BF(g)$ and $BF_2(g)$ were measured at ionizing electron energies slightly above appearance potentials (≈3 eV) in the temperature range 1477 to 1850 K and were used to obtain equilibrium data for the reaction $BF_3(g) + BF(g) = 2\ BF_2(g)$. We have analyzed their results and obtain $\Delta_r H°(298.15\ K) = 17.1 \pm 1.0\ kcal{\cdot}mol^{-1}$ from the 3rd law method with a drift of $-7.4 \pm 2.0\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ with JANAF heats of formation[2] for $BF_3(g)$ and $BF(g)$.

Although no other experimental determinations of enthalpy of formation of BF_2 have been reported, Margrave[3] combined the appearance potential of BF_2^+ from BF_3 of 16.5 eV with an estimated ionization potential for BF_2 (IP = 9.4 ± 0.1 eV)[4] and calculated $\Delta_f H°(BF_2, g) \leq -124 \pm 9\ kcal{\cdot}mol^{-1}$. Based on the JANAF value for $AP(BF_2^+)$ of 15.81 eV,[2] we calculate $\Delta_f H°(BF_2, g, 0\ K) = -141.3\ kcal{\cdot}mol^{-1}$ by the same method. Margrave[3] also derived $\Delta_f H° = -135\ kcal{\cdot}mol^{-1}$ *for* BF_2 *from average bond energy calculations and selected* $\Delta_f H°(BF_2, g) = -130 \pm 6\ kcal{\cdot}mol^{-1}$ as the 'best' value. It is now apparent that this value is several kilocalories too positive.

We note that the adopted enthalpy of formation leads to a progression in the stepwise bond dissociation energies for $BF(g)$, $BF_2(g)$ and $BF_3(g)$ which is consistent with the bond energy scheme predicted by Hildenbrand[5] for the Group III A fluorides, namely $D_1 > D_2 < D_3$. Using all JANAF data[2] we calculate bond dissociation energies of $D_1(B–F) = 179.4$, $D_2(BF–F) = 132.2$, and $D_3(BF_2–F) = 149.3\ kcal{\cdot}mol^{-1}$. The adopted value also corresponds to an ionization potential for BF_2 of 9.4 ± 0.2 eV[2] which appears reasonable in comparison with IP's for other Group III A dihalides[6] and is the value estimated for BF_2 by Steele *et al.*[4]

Heat Capacity and Entropy

Nelson and Gordy[7] were successful in producing trapped BF_2 radicals by gamma irradiation of *solid xenon which contained small* concentrations of BF_3. From observations on the electron spin resonance spectra of these radicals, a bond angle of 112° for BF_2 was derived by these workers to account for the hybridization of the α bonding orbitals of the boron atom. We adopt their result and assume the B–F bond length to be the same as that for BHF_2.[2] The three principal moments of inertia are: $I_A = 0.7385 \times 10^{-39}$, $I_B = 7.3289 \times 10^{-39}$, and $I_C = 8.0674 \times 10^{-39}\ g{\cdot}cm^2$.

The ground state electronic configuration ($^2A_1$) and doublet excited state ($^2B_1$) are estimated by analogy with those for NO_2.[8] The vibrational frequencies are calculated from the stretching and bending force constants of $k = 4.82 \times 10^5$ and $k\delta/l^2 = 0.84 \times 10^5$ dynes/cm by the valence force method. These force constants are estimated from those for CF_2 and SiF_2.[2]

References

[1] R. D. Srivastava and M. Farber, Trans. Faraday Soc. 67, 2298 (1971).

[2] JANAF Thermochemical Tables: $BF_3(g)$, 6–30–69; $BF(g)$, 12–31–64; $BF_2^+(g)$, 12–31–70; $BNF_2(g)$, 12–31–65; $CF_2(g)$, 6–30–70; $SiF_2(g)$, 12–31–68.

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[9] C. Thomson and D. Brotchie, Molec. Phys. 28, 301 (1974).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.617	−590.522	−590.522	INFINITE
100	33.582	207.676	280.540	−7.286	−590.123	−593.822	310.181
200	36.689	231.795	250.739	−3.789	−589.887	−597.632	156.085
250	38.629	240.188	247.813	−1.906	−589.878	−599.571	125.273
298.15	40.555	247.157	247.157	0.	−589.944	−601.433	105.369
300	40.629	247.408	247.157	0.075	−589.948	−601.504	104.731
350	42.585	253.819	247.659	2.156	−590.083	−603.420	90.056
400	44.409	259.626	248.798	4.331	−590.273	−605.313	79 046
450	46.050	264.953	250.301	6.594	−590.506	−607.179	70.480
500	47.494	269.882	252.015	8.933	−590.768	−609.018	63.624
600	49.827	278.757	255.749	13.805	−591.351	−612.614	53.333
700	51.554	286.575	259.606	18.878	−591.985	−616.109	45.975
800	52.837	293.547	263.421	24.101	−592.654	−619.510	40.450
900	53.801	299.828	267.123	29.435	−593.356	−622.825	36.148
1000	54.538	305.537	270.683	34.854	−594.090	−626.060	32.702
1100	55.111	310.763	274.092	40.337	−594.856	−629.220	29.879
1200	55.563	315.578	277.352	45.872	−595.656	−632.309	27.524
1300	55.925	320.040	280.466	51.447	−596.492	−635.330	25.528
1400	56.219	324.196	283.443	57.055	−597.364	−638.285	23.815
1500	56.461	328.083	286.291	62.689	−598.275	−641.176	22.328
1600	56.662	331.734	289.018	68.345	−599.223	−644.006	21.025
1700	56.831	335.174	291.633	74.020	−600.210	−646.775	19.873
1800	56.975	338.427	294.143	79.711	−601.234	−649.484	18.848
1900	57.100	341.510	296.555	85.415	−602.294	−652.136	17.928
2000	57.209	344.442	298.877	91.130	−603.387	−654.731	17.100
2100	57.306	347.236	301.114	96.856	−604.510	−657.271	16.349
2200	57.393	349.904	303.271	102.591	−605.662	−659.757	15.665
2300	57.474	352.457	305.355	108.334	−606.838	−662.189	15.039
2400	57.550	354.904	307.369	114.086	−658.293	−663.501	14.441
2500	57.622	357.255	309.317	119.844	−659.584	−663.692	13.867
2600	57.693	359.517	311.205	125.610	−660.855	−663.831	13.337
2700	57.762	361.695	313.035	131.383	−662.104	−663.922	12.844
2800	57.832	363.797	314.810	137.163	−663.327	−663.967	12.386
2900	57.903	365.828	316.535	142.949	−664.521	−663.968	11.959
3000	57.975	367.792	318.211	148.743	−665.683	−663.929	11.560
3100	58.048	369.694	319.841	154.544	−666.812	−663.852	11.186
3200	58.124	371.538	321.428	160.353	−667.904	−663.739	10.834
3300	58.202	373.328	322.974	166.169	−668.959	−663.593	10.504
3400	58.283	375.067	324.480	171.993	−669.974	−663.415	10.192
3500	58.365	376.757	325.950	177.826	−670.948	−663.207	9.898
3600	58.450	378.403	327.384	183.667	−671.881	−662.973	9.619
3700	58.538	380.005	328.785	189.516	−672.771	−662.713	9.356
3800	58.627	381.568	330.153	195.374	−673.619	−662.430	9.106
3900	58.718	383.092	331.491	201.241	−674.423	−662.125	8.868
4000	58.811	384.580	332.800	207.118	−675.184	−661.800	8.642
4100	58.904	386.033	334.081	213.004	−675.901	−661.456	8.427
4200	58.999	387.453	335.335	218.899	−1156.425	−654.071	8.135
4300	59.095	388.843	336.563	224.803	−1155.970	−642.116	7.800
4400	59.191	390.203	337.767	230.718	−1155.473	−630.172	7.481
4500	59.288	391.534	338.947	236.642	−1154.938	−618.239	7.176
4600	59.385	392.838	340.104	242.575	−1154.363	−606.319	6.885
4700	59.481	394.116	341.240	248.519	−1153.751	−594.411	6.606
4800	59.577	395.369	342.354	254.472	−1153.101	−582.517	6.339
4900	59.672	396.599	343.449	260.434	−1152.416	−570.637	6.083
5000	59.766	397.805	344.524	266.406	−1151.696	−558.771	5.837
5100	59.858	398.990	345.580	272.387	−1150.943	−546.920	5.602
5200	59.950	400.153	346.619	278.377	−1150.158	−535.084	5.375
5300	60.040	401.296	347.640	284.377	−1149.341	−523.263	5.157
5400	60.128	402.419	348.644	290.385	−1148.495	−511.458	4.947
5500	60.215	403.523	349.632	296.403	−1147.621	−499.670	4.745
5600	60.299	404.609	350.604	302.428	−1146.719	−487.896	4.551
5700	60.381	405.677	351.560	308.462	−1145.792	−476.140	4.363
5800	60.462	406.728	352.503	314.504	−1144.840	−464.401	4.182
5900	60.540	407.762	353.430	320.555	−1143.864	−452.677	4.008
6000	60.615	408.780	354.344	326.612	−1142.867	−440.970	3.839

PREVIOUS: June 1972 (1 atm) CURRENT: June 1972 (1 bar)

Difluoroborane, Ion (BF_2^+) IDEAL GAS $M_r = 48.806257$ Difluoroborane, Ion (BF_2^+) $B_1F_2^+$(g)

$S°(298.15\ K) = [225.1 \pm 1]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 315.8 \pm 2.5\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 322.6 \pm 2.5\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^1\Sigma_g^+$	0	1
$^1B_2$	[25000]	1

Vibrational Frequencies and Degeneracies

ν, cm^{-1}
[900](1)
[370](2)
[1550](1)

Point Group: [$D_{\infty h}$] σ = 2
Bond Distance: B–F = [1.31] Å
Bond Angle: F–B–F = [180]°
Rotational Constant: B_0 = [0.258528] cm^{-1}

Enthalpy of Formation

The electron impact reaction at low pressure in BF_3(g) has been studied with a mass spectrometer by Osberghaus,[1] Law[2] and Marriott.[3] From the reported appearance potentials 17.0 ± 0.5, 16.2 ± 0.2, and 16.7 ± 0.05 eV and assumed process $BF_3 + e = BF_2^+ + F + 2\ e$, we calculate the corresponding values of $\Delta_fH°(BF_2^+$, g, 298.15 K) as 104.5 ± 11.5, 86.1 ± 4.6, and 85.4 ± 1.2 kcal·mol^{-1}, using $\Delta_fH°(0\ K) = -170.747$ and 18.357 kcal·mol^{-1} for BF_3(g) and F(g). These electron impact values are superseded by the photoionization results of Dibeler and Liston[7] who report the onset of BF_2^+ from BF_3 as 15.81 eV (364.6 kcal·mol^{-1}). This yields $\Delta_fH°(0\ K) = 75.5 \pm 0.6$ kcal·mol^{-1} or $\Delta_fH°(298.15\ K) = 77.1 \pm 0.6$ kcal·mol^{-1}, which are adopted.

Heat Capacity and Entropy

The molecular structure is assumed to be linear using the Walsh[4] prediction for 16 valence electron XY_2 molecules. The electronic states, levels, and vibrational frequencies are estimated by comparison with those for CO_2.[5] The B–F bond distances is calculated by the method recommended by Krasnov.[5]

References

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[2] R. W. Law and J. L. Margrave, J. Chem. Phys. 25, 1086 (1956).
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[6] K. S. Krasnov, Zhur. Strukt. Khim. 1, 209 (1960).
[7] V. H. Dibeler and S. K. Liston, Inorg. Chem. 7, 1742 (1968).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−10.611	315.817		
100	31.424	184.214	260.803	−7.659			
200	39.162	208.493	229.047	−4.111			
250	42.008	217.548	225.865	−2.079			
298.15	44.291	225.148	225.148	0.	322.586	311.405	−54.557
300	44.371	225.422	225.149	0.082	322.628	311.335	−54.208
350	46.401	232.418	225.697	2.353	323.722	309.366	−46.170
400	48.172	238.732	226.938	4.718	324.761	307.244	−40.122
450	49.727	244.498	228.573	7.166	325.753	304.994	−35.403
500	51.091	249.809	230.435	9.687	326.712	302.636	−31.616
600	53.333	259.332	234.476	14.914	328.562	297.645	−25.912
700	55.047	267.688	238.636	20.336	330.357	292.350	−21.815
800	56.360	275.128	242.741	25.910	332.116	286.800	−18.726
900	57.375	281.827	246.718	31.598	333.848	281.032	−16.311
1000	58.168	287.915	250.538	37.377	335.553	275.071	−14.368
1100	58.794	293.489	254.193	43.226	337.231	268.942	−12.771
1200	59.296	298.627	257.684	49.132	338.880	262.661	−11.433
1300	59.702	303.390	261.019	55.082	340.499	256.243	−10.296
1400	60.035	307.827	264.206	61.070	342.084	249.702	−9.317
1500	60.311	311.979	267.254	67.088	343.636	243.049	−8.464
1600	60.541	315.879	270.172	73.131	345.152	236.294	−7.714
1700	60.736	319.555	272.970	79.195	346.634	229.445	−7.050
1800	60.901	323.031	275.656	85.277	348.080	222.509	−6.457
1900	61.043	326.328	278.236	91.374	349.492	215.494	−5.924
2000	61.165	329.462	280.720	97.485	350.873	208.406	−5.443
2100	61.272	332.449	283.113	103.607	352.224	201.249	−5.006
2200	61.365	335.302	285.421	109.739	353.548	194.029	−4.607
2300	61.446	338.031	287.649	115.879	354.848	186.749	−4.241
2400	61.519	340 648	289.803	122.028	305.868	180.482	−3.928
2500	61.583	343.161	291.888	128.183	307.052	175.233	−3.661
2600	61.640	345.577	293.907	134.344	308.255	169.936	−3.414
2700	61.692	347.905	295.864	140.511	309.479	164.593	−3.184
2800	61.739	350.149	297.763	146.682	310.727	159.204	−2.970
2900	61.782	352.316	299.607	152.858	312.001	153.770	−2.770
3000	61.821	354.411	301.399	159.038	313.303	148.292	−2.582
3100	61.858	356.439	303.142	165.222	314.636	142.770	−2.406
3200	61.893	358.404	304.838	171.410	316.001	137.204	−2.240
3300	61.925	360.309	306.490	177.601	317.400	131.595	−2.083
3400	61.956	362.158	308.100	183.795	318.833	125.943	−1.935
3500	61.986	363.954	309.671	189.992	320.302	120.249	−1.795
3600	62.016	365.701	311.203	196.192	321.808	114.512	−1.662
3700	62.045	367.400	312.699	202.395	323.350	108.732	−1.535
3800	62.074	369.055	314.160	208.601	324.928	102.911	−1.415
3900	62.103	370.668	315.589	214.810	326.544	97.047	−1.300
4000	62.133	372.241	316.985	221.022	328.198	91.142	−1 190
4100	62.163	373.775	318.352	227.237	329.888	85.194	−1.085
4200	62.194	375.274	319.689	233.454	−148.235	86.230	−1.072
4300	62.226	376.738	320.999	239.675	−145.385	91.778	−1 115
4400	62.259	378.169	322.282	245.900	−142.500	97.261	−1.155
4500	62.293	379.568	323.540	252.127	−139.582	102.677	−1.192
4600	62.328	380.938	324.773	258.358	−136.631	108.028	−1.227
4700	62.365	382.278	325.982	264.593	−133.649	113.315	−1.259
4800	62.402	383.592	327.169	270.831	−130.636	118.538	−1.290
4900	62.442	384.879	328.333	277.073	−127.592	123.697	−1.319
5000	62.482	386.141	329.477	283.320	−124.519	128.794	−1.346
5100	62.524	387.379	330.600	289.570	−121.418	133.830	−1.371
5200	62.568	388.593	331.704	295.825	−118.290	138.804	−1.394
5300	62.613	389.785	332.788	302.084	−115.136	143.718	−1.416
5400	62.659	390.956	333.855	308.347	−111.956	148.573	−1.437
5500	62.706	392.106	334.903	314.615	−108.752	153.368	−1.457
5600	62.755	393.237	335.935	320.888	−105.524	158.105	−1.475
5700	62.805	394.348	336.950	327.166	−102.274	162.783	−1.492
5800	62.856	395.440	337.949	333.449	−99.003	167.405	−1.508
5900	62.908	396.515	338.933	339.737	−95.711	171.970	−1.523
6000	62.961	397.573	339.901	346.031	−92.400	176.479	−1.536

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

Difluoroborane, Ion (BF_2^+) $B_1F_2^+$(g)

Difluoroborane, Ion (BF_2^-) IDEAL GAS $M_r = 48.807355$ Difluoroborane, Ion (BF_2^-) $B_1F_2^-(g)$

$S°(298.15\ K) = [240.7 \pm 2]\ J·K^{-1}·mol^{-1}$

$\Delta_fH°(0\ K) = -796.4 \pm 32\ kJ·mol^{-1}$

$\Delta_fH°(298.15\ K) = -802.1 \pm 32\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^1A_1$	0	1
$^3B_1$	[15000]	3
$^1B_1$	[35000]	1

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[1175](1)
[495](1)
[1188](1)

Point Group: $[C_{2v}]$ $\sigma = 2$

Bond Distance: B–F = [1.265] Å

Bond Angle: F–B–F = [100]°

Product of Moments of Inertia: $I_AI_BI_C = [3.74972 \times 10^{-116}]\ g^3·cm^6$

Enthalpy of Formation

The BF_2 ion has been detected mass spectrometrically by MacNeil and Thynne[1] and Farber *et al.*[2] MacNeil and Thynne[1] reported the formation of the negative ion at electron energies of approximately 7.6 eV as a result of electron bombardment of $BF_3(g)$. Assuming the ionization process to be $BF_3(g) + e = BF_2\ (g) + F(g)$, we calculate $\Delta_fH°(BF_2\ ,\ g,\ 0\ K) = -113.8\ kcal·mol^{-1}$ from their results with JANAF enthalpies of formation[3] for $BF_3(g)$ and F(g). This value leads to an unrealistic electron affinity (EA) for BF_2 of −1.1 eV. It seems most likely that the BF_2^- ion was formed in the dissociative ionization of $BF_3(g)$ with considerable excess energy.

Farber, *et al.*[2] observed the formation of the BF_2^- ion in a molecular flow effusion mass spectrometric study of the $BF_3(g) + KF(g) + B(cr)$ system. Equilibrium data for the electron transfer reaction $BF_2\ (g) + F(g) = BF_2(g) + F\ (g)$ were reported for the temperature range 1253 to 1640 K. We have analyzed their results with JANAF functions and obtain $\Delta_fH°(298.15\ K) = -26.3 \pm 1.8\ kcal·mol^{-1}$ by the 3rd law method with a drift of $-1.5 \pm 3.1\ cal·K^{-1}·mol^{-1}$, the 2nd law $\Delta_fH°(298.15\ K)$ value is $-24.2\ kcal·mol^{-1}$. We adopt the 3rd law value and calculate $\Delta_fH°(BF_2\ ,\ g,\ 298.15\ K) = -191.7 \pm 8.0\ kcal·mol^{-1}$ with JANAF auxiliary data. The adopted enthalpy of formation leads to EA $(BF_2) = 2.14 \pm 0.5$ eV.

Heat Capacity and Entropy

The correlation diagram of Walsh[4] predicts a bent configuration for BF_2^- (18 valence electrons) with a bond angle considerably reduced from that for $BF_2(112°)$.[3] These predictions are supported by the experimentally determined bond angles for the isoelectronic molecules $CF_2(104.9°)$,[3] $SiF_2(101°)$[3] and $GeF_2(94°)$.[5] Thus we adopt a bond angle for BF_2^- of 100° and assume the B–F bond length to be the same as that for BF.[3] The principal moments of inertia are: $I_A = 0.9240 \times 10^{-39}$, $I_B = 5.9251 \times 10^{-39}$, and $I_C = 6.8491 \times 10^{-39}\ g·cm^2$.

The electronic states, levels, and quantum weights are estimated by analogy with those for CF_2.[3] The vibrational frequencies are calculated form the stretching and bending force constants of $k = 5.16 \times 10^5$ and $k\delta/l^2 = 0.91 \times 10^5$ dynes/cn by the valence force method. These force constants are estimated by comparison with those for CF_2, SiF_2, and BF_2.[3]

References

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[3] JANAF Thermochemical Tables: $BF_3(g)$, 6–30–69; F(g), 9–30–65; $CF_2(g)$, 6–30–70; $SiF_2(g)$, 12–31–68, BF(g), 12–31–64; $BF_2(g)$, 6–30–72.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−10.609	−796.445		
100	33.599	201.283	274.065	−7.278			
200	36.676	225.419	244.310	−3.778			
250	38.519	233.799	241.394	−1.899			
298.15	40.352	240.740	240.740	0.	−802.073	−805.394	141.102
300	40.423	240.990	240.741	0.075	−802.115	−805.414	140.235
350	42.310	247.364	241.240	2.143	−803.302	−805.871	120.270
400	44.094	253.131	242.371	4.304	−804.547	−806.153	105.273
450	45.720	258.420	243.865	6.550	−805.835	−806.277	93.590
500	47.165	263.314	245.568	8.873	−807.153	−806.256	84.229
600	49.525	272.132	249.277	13.713	−809.846	−805.825	70.153
700	51.290	279.905	253.108	18.758	−812.586	−804.938	60.065
800	52.610	286 845	256.899	23.956	−815.359	−803.657	52.473
900	53.607	293.101	260.580	29.269	−818.160	−802.026	46.548
1000	54.372	298.791	264.121	34 670	−820.991	−800.082	41.792
1100	54.968	304.002	267.513	40.138	−823.851	−797.853	37.887
1200	55.439	308.806	270.756	45.659	−826.743	−795.362	34.621
1300	55.817	313.259	273.857	51.223	−829.669	−792.629	31.848
1400	56.124	317.407	276.821	56.820	−832.630	−789.669	29.463
1500	56.378	321.288	279.657	62 446	−835.628	−786.496	27.388
1600	56.591	324 934	282.374	68.095	−838.663	−783.121	25.566
1700	56.774	328.370	284.980	73.763	−841.735	−779.556	23.953
1800	56.933	331.620	287.482	79.449	−844.842	−775.809	22.513
1900	57.075	334.702	289.886	85.149	−847.984	−771.889	21.221
2000	57.207	337.633	292.201	90.863	−851.157	−767.801	20.053
2100	57.333	340.427	294.432	96.590	−854.358	−763.555	18.992
2200	57.457	343.097	296.583	102.330	−857.584	−759.156	18.025
2300	57.583	345.654	298.662	108.082	−860.829	−754.609	17.138
2400	57.713	348.107	300.671	113.847	−914.350	−748.852	16.298
2500	57.850	350.466	302.616	119.625	−917.700	−741.887	15.501
2600	57.995	352 738	304.500	125.417	−921.024	−734.789	14.762
2700	58.151	354.929	306.328	131.224	−924.317	−727.564	14.076
2800	58.319	357.047	308.102	137.048	−927.574	−720.217	13.436
2900	58.498	359.097	309.825	142.888	−930.793	−712.754	12.838
3000	58.689	361.083	311.501	148.748	−933 968	−705.182	12.278
3100	58.893	363.011	313.131	154.627	−937.098	−697.504	11.753
3200	59.108	364.884	314.719	160.526	−940.177	−689.726	11.259
3300	59.334	366.706	316.267	166.448	−943.205	−681.852	10.793
3400	59.570	368.481	317.777	172.394	−946.177	−673.887	10.353
3500	59.816	370.211	319.250	178.363	−949.093	−665.836	9.937
3600	60.070	371.900	320.690	184.357	−951.951	−657.702	9.543
3700	60.331	373.549	322.096	190.377	−954.750	−649.490	9.169
3800	60.597	375.162	323.471	196.423	−957.488	−641.203	8.814
3900	60.868	376.739	324.817	202.497	−960.164	−632.845	8.476
4000	61.142	378.284	326.134	208.597	−962 780	−624.419	8.154
4100	61.418	379.797	327.425	214.725	−965.334	−615.928	7.847
4200	61.694	381.280	328.690	220.881	−1447.676	−600.351	7.466
4300	61.970	382.735	329.930	227.064	−1449.020	−580.161	7.048
4400	62.244	384.163	331.146	233.275	−1450.307	−559.940	6.647
4500	62.515	385.565	332.340	239.513	−1451.535	−539.690	6.265
4600	62.782	386.942	333.512	245.778	−1452.708	−519.414	5.898
4700	63.045	388.295	334.663	252.069	−1453.826	−499.113	5.547
4800	63.302	389.625	335.794	258.386	−1454.891	−478.789	5.210
4900	63.552	390.933	336.906	264.729	−1455.904	−458.443	4.887
5000	63.795	392.219	338.000	271.096	−1456.867	−438.076	4.577
5100	64.031	393.485	339.075	277.488	−1457.782	−417.692	4.278
5200	64.258	394.730	340.134	283.902	−1458.652	−397.289	3.991
5300	64.477	395.956	341.175	290.339	−1459.476	−376.870	3.714
5400	64.687	397.163	342.201	296.797	−1460.259	−356.436	3.448
5500	64.887	398.352	343.211	303.276	−1461.002	−335.988	3.191
5600	65.078	399.523	344.206	309.775	−1461.706	−315.527	2.943
5700	65.260	400.677	345.187	316.292	−1462.374	−295.054	2.704
5800	65.431	401.813	346.153	322.826	−1463.008	−274.569	2.473
5900	65.593	402.933	347.106	329.377	−1463.611	−254.073	2.249
6000	65.745	404.037	348.046	335.944	−1464.183	−233.568	2.033

PREVIOUS: June 1972 (1 atm) CURRENT: June 1972 (1 bar)

Difluoroborane, Ion (BF_2^-) $B_1F_2^-(g)$

$S°(298.15\ K) = 244.0\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -730.3 \pm 3.3\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -733.9 \pm 3.3\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

υ, cm^{-1}	υ, cm^{-1}
2640(1)	1411 (1)
1174(1)	[1158](1)
544(1)	928 (1)

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: B–H = 1.15 Å; B–F = 1.30 ± 0.15 Å
Bond Angles: F–B–F = 120 ± 5°; F–B–H = 120 ± 2.5°
Product of the Moments of Inertia: $I_AI_BI_C = 7.51811 \times 10^{-116}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The equilibrium pressures at 296 and 360 K for the reaction 1/6 $B_2H_6(g) + 2/3\ BF_3(g) = HBF_2(g)$ were determined by Porter and Wason.[1] By the 3rd law method, the enthalpy change was evaluated to be 3.06 ± 0.33 kcal·mol^{-1}. Based on the values of $\Delta_fH°(298.15\ K)$ for $B_2H_6(g)$ and $BF_3(g)$ as 9.8 and −270.1 kcal·mol^{-1}, respectively, the enthalpy of formation for $BHF_2(g)$ was derived to be −175.4 ± 0.8 kcal·mol^{-1}. The drift in the 3rd law enthalpy of reaction is 3.6 cal·K^{-1}·mol^{-1}.

Heat Capacity and Entropy

The infrared spectrum of $BHF_2(g)$ has been observed by Coyle *et al.*,[2] Ritter, and Farrar,[2] Perec and Becks,[3] Lynds,[4] and Porter and Wason.[1]

The vibrational frequencies, except υ_5, were obtained form Porter and Wason[1] and corrected to the average isotopic species. The value of υ_5 was estimated by comparison with the same value reported by other investigators. The molecular structure, bond distances and angles were obtained from Perec and Becks.[3] The principal moments of inertia are: $I_A = 1.0402 \times 10^{-39}$, $I_B = 7.9974 \times 10^{-39}$, and $I_C = 9.0376 \times 10^{-39}$ g·cm^2.

The vibrational rotational spectrum of $BHF_2(g)$ has been studied by Lynds and Bass.[5] The values of υ_1, υ_2, υ_3, and υ_6 were assigned as 1164.2, 2620.8, 541.5 and 923.5 cm^{-1}, respectively, which are in fair agreement with the adopted values reported by Porter and Wason.[1]

References

[1] R. F. Porter and S. K. Wason, J. Phys. Chem. 69, 2208 (1965).
[2] T. D. Coyle, J. J. Ritter and T. C. Farrar, Proc. Chem. Soc. 25 (1964).
[3] M. Perec and L. N. Becks, J. Chem. Phys. 43, 721 (1965).
[4] L. Lynds, J. Chem. Phys. 42, 1124 (1965).
[5] L. Lynds and C. D. Bass, J. Chem Phys. 43, 4357 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−10.671	−730.272	−730.272	INFINITE
100	33.464	204.405	277.831	−7.343	−731.374	−729.711	381.162
200	36.674	228.378	247.707	−3.866	−732.506	−727.627	190.037
250	39.376	236.842	244.709	−1.967	−733.179	−726.330	151.758
298.15	42.358	244.029	244.029	0.	−733.874	−724.949	127.008
300	42.476	244.291	244.030	0.078	−733.901	−724.893	126.215
350	45.706	251.082	244.559	2.283	−734.637	−723.334	107.952
400	48.856	257.392	245.773	4.648	−735.366	−721.669	94.240
450	51.806	263.319	247.396	7.165	−736.074	−719.914	83.565
500	54.504	268.919	249.271	9.824	−736.748	−718.082	75.018
600	59.136	279.281	253.424	15.514	−737.977	−714.231	62.179
700	62.868	288.688	257.800	21.621	−739.046	−710.187	52.995
800	65.882	297.286	262.206	28.064	−739.971	−705.999	46.097
900	68.332	305.192	266.549	34.779	−740.780	−701.703	40.726
1000	70.340	312.499	270.783	41.716	−741.497	−697.322	36.424
1100	71.997	319.283	274.888	48.835	−742.147	−692.873	32.902
1200	73.374	325.609	278.854	56.106	−742.750	−688.366	29.964
1300	74.528	331.529	282.681	63.503	−743.325	−683.811	27.476
1400	75.500	337.089	286.370	71.005	−743.884	−679.212	25.342
1500	76.325	342.326	289.928	78.598	−744.441	−674.573	23.491
1600	77.030	347.275	293.359	86.266	−745.003	−669.897	21.870
1700	77.636	351.964	296.670	94.000	−745.577	−665.185	20.439
1800	78.159	356.417	299.866	101.791	−746.168	−660.439	19.165
1900	78.614	360.655	302.955	109.630	−746.779	−655.660	18.025
2000	79.011	364.698	305.942	117.512	−747.411	−650.848	16.998
2100	79.360	368.561	308.832	125.431	−748.064	−646.004	16.068
2200	79.667	372.260	311.632	133.382	−748.738	−641.128	15.222
2300	79.940	375.808	314.346	141.363	−749.432	−636.221	14.449
2400	80.182	379.215	316.978	149.369	−800.403	−630.215	13.716
2500	80.399	382.493	319.534	157.398	−801.209	−623.107	13.019
2600	80.593	385.650	322.016	165.448	−801.995	−615.968	12.375
2700	80.767	388.695	324.430	173.516	−802.760	−608.798	11.778
2800	80.925	391.635	326.778	181.601	−803.503	−601.601	11.223
2900	81.068	394.477	329.063	189.701	−804.221	−594.377	10.706
3000	81.197	397.228	331.290	197.814	−804.912	−587.129	10.223
3100	81.315	399.892	333.460	205.940	−805.576	−579.859	9.771
3200	81.423	402.476	335.577	214.077	−806.211	−572.568	9.346
3300	81.522	404.983	337.642	222.224	−806.816	−565.257	8.947
3400	81.612	407.418	339.659	230.381	−807.391	−557.928	8.572
3500	81.695	409.785	341.629	238.546	−807.935	−550.583	8.217
3600	81.772	412.087	343.554	246.720	−808.447	−543.223	7.882
3700	81.843	414.329	345.437	254.901	−808.928	−535.848	7.565
3800	81.908	416.512	347.279	263.088	−809.378	−528.462	7.264
3900	81.969	418.641	349.081	271.282	−809.798	−521.064	6.979
4000	82.025	420.717	350.846	279.482	−810.186	−513.655	6.708
4100	82.078	422.743	352.575	287.687	−810.545	−506.238	6.450
4200	82.127	424.721	354.269	295.897	−1290.723	−491.787	6.116
4300	82.172	426.654	355.930	304.112	−1289.936	−472.775	5.743
4400	82.215	428.544	357.559	312.332	−1289.123	−453.780	5.387
4500	82.255	430.392	359.157	320.555	−1288.284	−434.804	5.047
4600	82.292	432.200	360.726	328.783	−1287.421	−415.848	4.722
4700	82.328	433.970	362.265	337.014	−1286.534	−396.910	4.411
4800	82.361	435.704	363.777	345.248	−1285.625	−377.991	4.113
4900	82.392	437.403	365.263	353.486	−1284.695	−359.092	3.828
5000	82.421	439.067	366.722	361.726	−1283.744	−340.211	3.554
5100	82.448	440.700	368.157	369.970	−1282.773	−321.351	3.291
5200	82.475	442.301	369.567	378.216	−1281.785	−302.508	3.039
5300	82.499	443.872	370.954	386.465	−1280.778	−283.686	2.796
5400	82.522	445.415	372.319	394.716	−1279.755	−264.882	2.562
5500	82.545	446.929	373.662	402.969	−1278.716	−246.098	2.337
5600	82.565	448.416	374.984	411.225	−1277.663	−227.332	2.120
5700	82.585	449.878	376.285	419.482	−1276.595	−208.586	1.911
5800	82.604	451.314	377.566	427.742	−1275.514	−189.859	1.710
5900	82.622	452.727	378.828	436.003	−1274.420	−171.150	1.515
6000	82.639	454.116	380.071	444.266	−1273.314	−152.460	1.327

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

Difluorohydroxyborane (BF_2OH) IDEAL GAS M_r = 65.814146 Difluorohydroxyborane (BF_2OH) $B_1F_2H_1O_1(g)$

$S°(298.15\ K) = [269.17]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [-1077 \pm 20]\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = [-1084 \pm 20]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}
[3680](1)	[888](1)
[1463](1)	[696](1)
[1420](1)	[480](1)
[1250](1)	[480](1)
[1250](1)	

Ground State Quantum Weight: 1 $\sigma = 1$

Point Group: C_s

Bond Distances: B–F = [1.30] Å; B–O = [1.36] Å; O–H = [0.96] Å

Bond Angles: F–B–F = [120]°; F–B–O = [120]°; B–O–H = [105]°

Product of the Moments of Inertia: $I_A I_B I_C = [1.051510 \times 10^{-114}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The value of enthalpy of formation, $\Delta_f H°(298.15\ K)$, was calculated based on an assumption that $\Delta_r H°(298.15\ K) = 0$ for the reaction 2/3 $BF_3(g)$ + 1/3 $B(OH)_3(g) = BOHF_2(g)$.

Heat Capacity and Entropy

The vibrational frequencies were obtained from Gordon.[1] The B–F and O–H bond distances were assumed to be the same as those in $BF_3(g)$ and $H_2O(g)$ molecules, respectively. The B–O bond distance and the bond angles were estimated from related molecules The principal moments of inertia are: $I_A = 7.8128 \times 10^{-39}$, $I_B = 8.3349 \times 10^{-39}$, and $I_C = 16.1476 \times 10^{-39}\ g{\cdot}cm^2$.

Reference

[1] J. S. Gordon, Astrosystems International, Inc. (1962).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−11.726	−1076.768	−1076.768	INFINITE
100	34.095	224.715	308.596	−8.388	−1079.313	−1071.015	559.441
200	42.159	250.509	273.610	−4.620	−1081.609	−1061.807	277.316
250	47.167	260.453	270.002	−2.387	−1082.677	−1056.732	220.792
298.15	51.982	269.174	269.174	0.	−1083.656	−1051.646	184.244
300	52.164	269.496	269.175	0.096	−1083.692	−1051.447	183.073
350	56.990	277.902	269.828	2.826	−1084.641	−1045.997	156.106
400	61.514	285.812	271.336	5.790	−1085.519	−1040.415	135.864
450	65.653	293.300	273.364	8.971	−1086.322	−1034.728	120.108
500	69.373	300.413	275.716	12.349	−1087.048	−1028.956	107.494
600	75.605	313.636	280.952	19.610	−1088.285	−1017.217	88.557
700	80.471	325.671	286.494	27.424	−1089.275	−1005.291	75.016
800	84.305	336.676	292.089	35.670	−1090.065	−993.237	64.852
900	87.380	346.790	297.613	44.260	−1090.702	−981.094	56.941
1000	89.894	356.131	303.003	53.127	−1091.219	−968.887	50.609
1100	91.983	364.799	308.232	62.224	−1091.646	−956.632	45.427
1200	93.744	372.881	313.286	71.513	−1092.006	−944.342	41.106
1300	95.244	380.445	318.165	80.964	−1092.317	−932.023	37.449
1400	96.532	387.552	322.870	90.555	−1092.596	−919.683	34.314
1500	97.647	394.251	327.407	100.265	−1092.855	−907.323	31.596
1600	98.617	400.584	331.785	110.079	−1093.105	−894.946	29.217
1700	99.465	406.589	336.010	119.984	−1093.354	−882.553	27.118
1800	100.210	412.296	340.091	129.969	−1093.609	−870.146	25.251
1900	100.868	417.732	344.035	140.024	−1093.874	−857.724	23.580
2000	101.451	422.921	347.851	150.140	−1094.152	−845.288	22.077
2100	101.969	427.883	351.544	160.312	−1094.446	−832.838	20.716
2200	102.432	432.638	355.123	170.532	−1094.755	−820.373	19.478
2300	102.847	437.200	358.593	180.796	−1095.081	−807.893	18.348
2400	103.219	441.585	361.960	191.100	−1145.681	−794.331	17.288
2500	103.554	445.806	365.230	201.439	−1146.114	−779.683	16.291
2600	103.857	449.873	368.408	211.810	−1146.527	−765.017	15.369
2700	104.132	453.798	371.499	222.210	−1146.920	−750.336	14.516
2800	104.382	457.590	374.506	232.635	−1147.290	−735.641	13.724
2900	104.609	461.257	377.434	243.085	−1147.637	−720.933	12.985
3000	104.817	464.807	380.288	253.557	−1147.959	−706.213	12.296
3100	105.007	468.247	383.070	264.048	−1148.255	−691.484	11.651
3200	105.182	471.584	385.784	274.558	−1148.524	−676.745	11.047
3300	105.342	474.823	388.434	285.084	−1148.766	−661.998	10.479
3400	105.490	477.970	391.021	295.626	−1148.979	−647.244	9.944
3500	105.626	481.030	393.549	306.182	−1149.164	−632.485	9.439
3600	105.753	484.007	396.021	316.751	−1149.321	−617.720	8.963
3700	105.870	486.906	398.438	327.332	−1149.449	−602.951	8.512
3800	105.978	489.731	400.803	337.924	−1149.548	−588.180	8.085
3900	106.079	492.485	403.119	348.527	−1149.620	−573.405	7.680
4000	106.173	495.172	405.387	359.140	−1149.663	−558.630	7.295
4100	106.260	497.795	407.609	369.761	−1149.679	−543.854	6.929
4200	106.342	500.356	409.787	380.392	−1629.519	−522.054	6.493
4300	106.419	502.860	411.922	391.030	−1628.395	−495.699	6.022
4400	106.490	505.307	414.017	401.675	−1627.249	−469.371	5.572
4500	106.558	507.701	416.072	412.328	−1626.080	−443.068	5.143
4600	106.621	510.043	418.090	422.987	−1624.890	−416.793	4.733
4700	106.680	512.337	420.071	433.652	−1623.681	−390.542	4.340
4800	106.736	514.584	422.017	444.323	−1622.453	−364.318	3.965
4900	106.789	516.785	423.928	454.999	−1621.208	−338.120	3.604
5000	106.838	518.943	425.807	465.680	−1619.947	−311.947	3.259
5100	106.885	521.059	427.654	476.366	−1618.671	−285.800	2.927
5200	106.929	523.135	429.470	487.057	−1617.381	−259.678	2.608
5300	106.971	525.172	431.257	497.752	−1616.080	−233.580	2.302
5400	107.011	527.172	433.015	508.451	−1614.768	−207.508	2.007
5500	107.049	529.136	434.744	519.154	−1613.447	−181.460	1.723
5600	107.085	531.065	436.447	529.861	−1612.118	−155.435	1.450
5700	107.118	532.961	438.124	540.571	−1610.782	−129.435	1.186
5800	107.151	534.824	439.775	551.285	−1609.440	−103.458	0.932
5900	107.181	536.656	441.402	562.001	−1608.095	−77.505	0.686
6000	107.211	538.458	443.004	572.721	−1606.746	−51.574	0.449

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

Difluorohydroxyborane (BF_2OH) $B_1F_2H_1O_1(g)$

Boron Fluoride Oxide (OBF$_2$) IDEAL GAS $M_r = 64.806206$ Boron Fluoride Oxide (OBF$_2$) $B_1F_2O_1(g)$

$S°(298.15\ K) = [267.8]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [-834 \pm 15]\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = [-837 \pm 15]\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights	
ϵ_i, cm^{-1}	g_i
0	[2]
17171	[2]
22390	[2]

Vibrational Frequencies and Degeneracies	
ν, cm^{-1}	ν, cm^{-1}
1377(1)	[850](1)
856(1)	[1100](1)
491(1)	[500](1)

Point Group: C_{2v} $\sigma = 2$
Bond Distances: B–F = 1.30 ± 0.05 Å; B–O = 1.40 ± 0.05 Å
Bond Angles: F–B–O = 117 ± 5°; F–B–F = 126 ± 5°
Product of the Moments of Inertia: $I_AI_BI_C = 9.948921 \times 10^{-115}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The molecule $BF_2O(g)$ is similar to $BO_2(g)$ in that both have an extra electron. Based on an assumption that $D_0°(F_2B–O) = D_0°(OB–O) - 10 = 134.3\ kcal{\cdot}mol^{-1}$ where the quantity $\sim 10\ kcal{\cdot}mol^{-1}$ is estimated as the resonance stabilization energy in $BO_2(g)$, $\Delta_fH°(F_2BO, g, 298.15\ K)$ is calculated to be $-206\ kcal{\cdot}mol^{-1}$.

Assuming $D_0°(F_2BO–H) = D_0°(HO–H) = 118\ kcal{\cdot}mol^{-1}$, the value of $\Delta_fH°(F_2BO, g, 298.15\ K)$ is evaluated as $-191.6\ kcal{\cdot}mol^{-1}$, using $\Delta_fH°(0\ K) = 51.63$ and $-257.35\ kcal{\cdot}mol^{-1}$ for H(g) and $F_2BOH(g)$, respectively.

The value of $\Delta_fH°(F_2BO, g, 298.15\ K)$ is tentatively adopted as $-200 \pm 15\ kcal{\cdot}mol^{-1}$

Heat Capacity and Entropy

The 4465–A emission spectrum was observed in a discharge through BF_3 and O_2 by Mathews.[1] The emitter of the discharge was shown to be either the planar BOF_2 molecule or molecule–ion BOF_2^{+}. No experimental evidence has been found to distinguish between them. The molecular structure, bond distances and angles were reported by Mathews,[1] based on a rotational analysis of the emission spectrum. These values are adopted here.

Three vibrational frequencies for both $^{11}B^{16}OF_2$ and $^{10}B^{16}OF_2$ molecules (or ions) were deermined by vibrational analysis of the 5800–Å bands of the emission spectrum by Mathews and Innes.[2] These values are corrected to the average isotopic species and adopted. The last three frequencies are estimated from values calculated by the valence–force method, using force constants transferred from $COF_2(g)$.

The ground state quantum weight is taken as 2 because of the extra electron. The other two electronic levels are estimated from the band systems at 5800 and 4465 Å, assuming that two systems have a common lower state, i.e. the ground state.

The principal moments of inertia are: $I_A = 7.4051 \times 10^{-39}$, $I_B = 8.4655 \times 10^{-39}$, and $I_C = 15.8706 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] C. W. Mathews, J. Mol. Spectry. 19, 203 (1966).
[2] C. W. Mathews and K. K. Innes, J. Mol. Spectry. 15, 199 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−11.535	−833.955	−833.955	INFINITE
100	33.949	224.266	306.266	−8.200	−835.003	−831.696	434.434
200	41.185	249.703	272.146	−4.489	−836.009	−827.987	216.248
250	45.839	259.392	268.645	−2.313	−836.436	−825.931	172.569
298.15	50.199	267.842	267.842	0.	−836.800	−823.874	144.339
300	50.360	268.153	267.843	0.093	−836.813	−823.794	143.435
350	54.500	276.233	268.472	2.716	−837.144	−821.597	122.617
400	58.160	283.755	269.918	5.535	−837.438	−819.355	106.997
450	61.331	290.793	271.850	8.524	−837.703	−817.079	94.844
500	64.045	297.399	274.078	11.660	−837.939	−814.774	85.119
600	68.325	309.475	278.991	18.290	−838.344	−810.102	70.526
700	71.432	320.254	284.130	25.287	−838.682	−805.368	60.097
800	73.715	329.949	289.262	32.550	−838.979	−800.588	52.273
900	75.422	338.734	294.278	40.010	−839.257	−795.772	46.185
1000	76.721	346.751	299.131	47.620	−839.530	−790.926	41.314
1100	77.729	354.113	303.799	55.345	−839.810	−786.052	37.327
1200	78.523	360.911	308.279	63.159	−840.105	−781.152	34.003
1300	79.158	367.222	312.573	71.044	−840.422	−776.227	31.189
1400	79.674	373.108	316.689	78.987	−840.767	−771.276	28.777
1500	80.097	378.620	320.636	86.976	−841.143	−766.299	26.685
1600	80.449	383.801	324.424	95.004	−841.554	−761.297	24.854
1700	80.744	388.687	328.061	103.064	−842.001	−756.267	23.237
1800	80.994	393.310	331.559	111.151	−842.487	−751.210	21.800
1900	81.209	397.695	334.926	119.261	−843.009	−746.125	20.512
2000	81.394	401.865	338.169	127.392	−843.569	−741.011	19.353
2100	81.557	405.840	341.298	135.540	−844.163	−735.869	18.304
2200	81.700	409.638	344.318	143.702	−844.791	−730.698	17.349
2300	81.829	413.272	347.238	151.879	−845.449	−725.497	16.477
2400	81.945	416.757	350.062	160.068	−896.393	−719.198	15.653
2500	82.053	420.105	352.798	168.268	−897.180	−711.799	14.872
2600	82.153	423.325	355.449	176.478	−897.955	−704.369	14.151
2700	82.249	426.427	358.020	184.698	−898.715	−696.908	13.483
2800	82.341	429.420	360.517	192.928	−899.457	−689.420	12.861
2900	82.431	432.311	362.943	201.166	−900.178	−681.906	12.282
3000	82.520	435.107	365.302	209.414	−900.875	−674.368	11.742
3100	82.610	437.814	367.598	217.671	−901.546	−666.806	11.236
3200	82.701	440.439	369.834	225.936	−902.188	−659.224	10.761
3300	82.793	442.985	372.012	234.211	−902.800	−651.622	10.314
3400	82.888	445.458	374.136	242.495	−903.379	−644.001	9.894
3500	82.985	447.862	376.208	250.788	−903.924	−636.365	9.497
3600	83.085	450.201	378.231	259.092	−904.434	−628.713	9.122
3700	83.189	452.479	380.207	267.405	−904.907	−621.047	8.768
3800	83.296	454.699	382.138	275.730	−905.343	−613.369	8.431
3900	83.407	456.864	384.027	284.065	−905.740	−605.680	8.112
4000	83.521	458.977	385.874	292.411	−906.099	−597.982	7.809
4100	83.639	461.041	387.683	300.769	−906.418	−590.275	7.520
4200	83.760	463.058	389.453	309.139	−1386.548	−575.536	7.158
4300	83.884	465.030	391.188	317.521	−1385.702	−556.237	6.757
4400	84.011	466.960	392.888	325.916	−1384.818	−536.957	6.374
4500	84.141	468.850	394.555	334.324	−1383.898	−517.698	6.009
4600	84.273	470.700	396.191	342.744	−1382.941	−498.460	5.660
4700	84.408	472.514	397.795	351.178	−1381.949	−479.242	5.326
4800	84.544	474.293	399.371	359.626	−1380.923	−460.046	5.006
4900	84.682	476.037	400.917	368.087	−1379.863	−440.872	4.700
5000	84.822	477.750	402.437	376.563	−1378.770	−421.720	4.406
5100	84.962	479.431	403.930	385.052	−1377.646	−402.590	4.123
5200	85.103	481.082	405.398	393.555	−1376.492	−383.483	3.852
5300	85.244	482.704	406.841	402.072	−1375.309	−364.397	3.591
5400	85.385	484.299	408.261	410.604	−1374.099	−345.335	3.340
5500	85.526	485.867	409.658	419.149	−1372.863	−326.296	3.099
5600	85.667	487.409	411.033	427.709	−1371.604	−307.278	2.866
5700	85.806	488.927	412.386	436.283	−1370.321	−288.284	2.642
5800	85.945	490.420	413.718	444.870	−1369.017	−269.312	2.425
5900	86.082	491.891	415.031	453.472	−1367.694	−250.363	2.217
6000	86.218	493.339	416.324	462.087	−1366.354	−231.437	2.015

PREVIOUS: December 1966 (1 atm) CURRENT· December 1966 (1 bar)

Trifluoroborane (BF_3) **IDEAL GAS** **M_r = 67.805209** **Trifluoroborane (BF_3)** **$B_1F_3(g)$**

$S°(298.15 K) = 254.36 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0 K) = -1132.8 \pm 1.7\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15 K) = -1135.6 \pm 1.7\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
888 (1)
696.7 (1)
1463.3 (2)
480.7 (2)

Ground State Quantum Weight: 1 $\sigma = 6$
Point Group: D_{3h}
Bond Distance: B–F = 1.307 ± 0.002 Å
Bond Angle: F–B–F = 120°
Products of the Moments of Inertia: $I_AI_BI_C = 1.056517 \times 10^{-114}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The adopted enthalpy of formation was selected by a simultaneous adjustment of several interrelated pieces of data relating to the heat of formation of HF (see HF, g table 12–31–68). The data which were considered relating directly to BF_3 were as follows:

A. $NF_3(g) + B(cr, \beta) \rightarrow BF_3(g) + 0.5\ N_2$ and $\Delta_rH°(298.15 K) = 239.46 \pm 1.2\ kcal{\cdot}mol^{-1}$.

Ludwig and Cooper[1] report the above value after corretion for 0 44 percent impurities in the boron. As much as 5 percent unburned boron was determined by analysis.

B. $1.5\ F_2(g) + B(cr, \beta) \rightarrow BF_3(g)$

Wise *et al.*[2] originally reported $\Delta_rH°(298.15 K) = -270.1 \pm 0.24\ kcal{\cdot}mol^{-1}$ but later reanalysis [3] of the impurities and due allowance for their effect changed this to $-271.6 \pm 0.9\ kcal{\cdot}mol^{-1}$. Johnson *et al.*[3] using zone refined boron obtained $\Delta_rH°(298.15 K) = -271.65 \pm 0.22\ kcal{\cdot}mol^{-1}$ after correction for 0.12 percent impurities. Domalski and Armstrong[4] obtained $\Delta_rH°(298.15 K) = -271.03 \pm 0.51\ kcal{\cdot}mol^{-1}$ from a combustion in the presence of Teflon, the boron contained 0.32 percent impurities and corrections were included. The above reaction constituted about 0.35 of the total energy measured. The measurements of Gross *et al.*,[5] although on a zone refined sample, did not include a complete purity analysis and their data were not included since probable impurities could introduce serious errors.

C. $3\ HF(50\ H_2O) + B(cr, \beta) + 0.75\ O_2(g) \rightarrow BF_3(g) + 1.5\ H_2O(l)$

From the measurements of Gunn[6] on the reaction of $BF_3(g) + 15.67\ HF(3.747\ H_2O) \rightarrow$ [solution] and Good and Mansson[7] for the reaction $B(cr, \beta) + 0.75\ O_2(g) + 18.57\ HF(3.065\ H_2O) \rightarrow$ [solution] $+ 1.5\ H_2O(l)$, where the resulting solutions have the same composition, we obtain $\Delta_rH°(298.15 K) = -142.77 \pm 0.5\ kcal{\cdot}mol^{-1}$. Further details of the simultaneous solution are given by Syverud.[8]

Heat Capacity and Entropy

The fundamental frequencies were selected from the measurements of Lindeman and Wilson,[9] McKean,[10] Nielsen,[11] Anderson *et al.*[12] and Yost *et al.*[13] The bond length and structure of those reported by Gin *et al.*[14] which are in agreement with those of Kuchitsu and Konaka[15] from gas phase electron diffraction. These measurements disagree with the earlier determinations of Nielsen[11] and Levy and Brockway[16] but are considerably more precise and are adopted.

The principal moments of inertia are $I_A = I_B = 8.0838 \times 10^{-39}$, and $I_C = 16.1676 \times 10^{-39}\ g{\cdot}cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−11.647	−1132.817	−1132.817	INFINITE
100	34.089	210.208	293.304	−8.310	−1133.864	−1129.299	589.885
200	41.964	235.971	258.706	−4.547	−1134.828	−1124.343	293.648
250	46.471	245.824	255.164	−2.335	−1135.240	−1121.673	234.361
298.15	50.446	254.355	254.355	0.	−1135.621	−1119.025	196.049
300	50.590	254.668	254.356	0.093	−1135.636	−1118.922	194.822
350	54.273	262.749	254.986	2.717	−1136.023	−1116.106	166.570
400	57.539	270.213	256.429	5.514	−1136.407	−1113.235	145.374
450	60.420	277.160	258.351	8.464	−1136.785	−1110.315	128.882
500	62.945	283.660	260.560	11.550	−1137.150	−1107.355	115.685
600	67.071	295.518	265.418	18.060	−1137.831	−1101.330	95.879
700	70.195	306.103	270.488	24.931	−1138.443	−1095.198	81.725
800	72.569	315.638	275.546	32.074	−1138.997	−1088.981	71.103
900	74.389	324.295	280.489	39.426	−1139.508	−1082.698	62.838
1000	75.802	332.209	285.271	46.938	−1139.993	−1076.360	56.223
1100	76.914	339.488	289.873	54.576	−1140.465	−1069.974	50.809
1200	77.800	346.220	294.292	62.314	−1140.935	−1063.545	46.295
1300	78.516	352.476	298.530	70.131	−1141.413	−1057.076	42.474
1400	79.101	358.317	302.594	78.013	−1141.907	−1050.570	39.197
1500	79.584	363.792	306.493	85.948	−1142.422	−1044.028	36.356
1600	79.988	368.941	310.237	93.927	−1142.963	−1037.451	33.869
1700	80.327	373.801	313.834	101.943	−1143.531	−1030.840	31.674
1800	80.616	378.401	317.295	109.991	−1144.127	−1024.194	29.721
1900	80.863	382.766	320.627	118.065	−1144.752	−1017.514	27.973
2000	81.076	386.919	323.838	126.162	−1145.404	−1010.800	26.399
2100	81.261	390.880	326.937	134.279	−1146.080	−1004.054	24.974
2200	81.423	394.664	329.930	142.413	−1146.777	−997.274	23.678
2300	81.564	398.286	332.824	150.563	−1147.491	−990.462	22.494
2400	81.689	401.760	335.625	158.726	−1198.477	−982.551	21.385
2500	81.800	405.097	338.337	166.900	−1199.289	−973.537	20.341
2600	81.899	408.308	340.967	175.085	−1200.072	−964.492	19.377
2700	81.988	411.400	343.519	183.280	−1200.822	−955.416	18.484
2800	82.067	414.383	345.997	191.483	−1201.536	−946.314	17.654
2900	82.139	417.265	348.405	199.693	−1202.209	−937.187	16.881
3000	82.203	420.050	350.747	207.910	−1202.839	−928.038	16.159
3100	82.262	422.747	353.026	216.133	−1203.422	−918.868	15.483
3200	82.315	425.359	355.246	224.362	−1203.957	−909.680	14.849
3300	82.364	427.893	357.409	232.596	−1204.442	−900.476	14.253
3400	82.408	430.352	359.519	240.835	−1204.875	−891.259	13.693
3500	82.449	432.742	361.577	249.078	−1205.255	−882.029	13.164
3600	82.487	435.065	363.586	257.325	−1205.581	−872.789	12.664
3700	82.521	437.326	365.549	265.575	−1205.852	−863.541	12.191
3800	82.553	439.527	367.466	273.829	−1206.069	−854.286	11.743
3900	82.583	441.671	369.342	282.086	−1206.232	−845.026	11.318
4000	82.610	443.763	371.176	290.346	−1206.341	−835.763	10.914
4100	82.636	445.803	372.972	298.608	−1206.396	−826.498	10.530
4200	82.660	447.794	374.730	306.873	−1686.248	−810.208	10.076
4300	82.682	449.740	376 451	315.140	−1685.110	−789.364	9.589
4400	82.702	451.641	378.139	323.409	−1683.924	−768.546	9.124
4500	82.721	453.500	379.793	331.680	−1682.689	−747.755	8.680
4600	82.739	455.318	381.415	339.953	−1681.408	−726.993	8.255
4700	82.756	457.097	383.006	348.228	−1680.081	−706.259	7.849
4800	82.772	458.840	384.568	356.504	−1678.710	−685.554	7.460
4900	82.787	460.547	386.101	364.782	−1677.297	−664.878	7.088
5000	82.801	462.219	387.607	373.062	−1675.842	−644.231	6.730
5100	82.814	463.859	389.086	381.343	−1674.349	−623.613	6.387
5200	82.827	465.468	390.540	389.625	−1672.817	−603.025	6.057
5300	82.839	467.045	391.968	397.908	−1671.249	−582.467	5.741
5400	82.850	468.594	393.373	406.192	−1669.647	−561.939	5.436
5500	82.860	470.114	394.755	414.478	−1668.011	−541.442	5.142
5600	82.870	471.607	396.114	422.764	−1666.344	−520.973	4.859
5700	82.880	473.074	397.451	431.052	−1664.647	−500.536	4.587
5800	82.889	474.516	398.767	439.340	−1662.921	−480.128	4.324
5900	82.897	475.933	400.063	447.630	−1661.168	−459.749	4.070
6000	82.905	477.326	401.339	455.920	−1659.389	−439.401	3.825

PREVIOUS June 1969 (1 atm) CURRENT: June 1969 (1 bar)

Trifluoroborane (BF_3) **$B_1F_3(g)$**

Potassium Tetrafluoroborate (KBF_4) CRYSTAL(I–II) $M_r = 125.901912$ Potassium Tetrafluoroborate (KBF_4) $B_1F_4K_1(cr)$

$\Delta_fH°(0\ K)$ = Unknown
$S°(298.15\ K) = 133.89 \pm 4.0\ J\ K^{-1}\cdot mol^{-1}$
$\Delta_fH°(298.15\ K) = -1887 \pm 4\ kJ\cdot mol^{-1}$
$T_{trs} = 556\ K$
$\Delta_{trs}H° = 14.06 \pm 0.16\ kJ\cdot mol^{-1}$
$T_{fus} = 843\ K$
$\Delta_{fus}H° = 17.66 \pm 0.16\ kJ\cdot mol^{-1}$

Enthalpy of Formation

Bills and Cotton[1] measured the enthalpies of several reactions at 25°C which led to the following result:

$H_3BO_3(cr) + 4(HF23\ H_2O) + KNO_3(cr) \rightarrow KBF_4(cr) + HNO_392\ H_2O + 3\ H_2O$.

Combining this result with the following enthalpy of formation data,

$\Delta_fH°(H_3BO_3, cr) = -261.47 \pm 0.2\ kcal\cdot mol^{-1}$ [2]
$\Delta_fH°(HF23\ H_2O) = -76.75 \pm 0.1\ kcal\cdot mol^{-1}$ [3]
$\Delta_fH°(KNO_3, cr) = -118.22\ kcal\cdot mol^{-1}$ [4]
$\Delta_fH°(HNO_392\ H_2O) = -49.44\ kcal\cdot mol^{-1}$ [5]
$\Delta_fH°(H_2O, l) = -68.315\ kcal\cdot mol^{-1}$

We derive, $\Delta_fH°(KBF_4, cr) = -451.6 \pm 1.2\ kcal\cdot mol^{-1}$.

Gross, Hayman and Joel[6] recently measured the following enthalpies of reaction:

$NaF(cr) + BF_3(g) \rightarrow NaBF_4(cr)$ $\Delta_rH° = -32.04 \pm 0.12\ kcal\cdot mol^{-1}$
$[KBF_4 + NaF](cr) + HF(aq) \rightarrow$ Soln A $\Delta_{sol}H° = +8.14 \pm 0.18\ kcal\cdot mol^{-1}$
$[NaBF_4 + KF](cr) + HF(aq) \rightarrow$ Soln A $\Delta_{sol}H° = -2.94 \pm 0.13\ kcal\cdot mol^{-1}$

These data combine to give $\Delta H_r = -43.13 \pm 0.22\ kcal\cdot mol^{-1}$ for the reaction $KF(cr) + BF_3(g) \rightarrow KBF_4(cr)$ Combining this result with the following enthalpies of formation: $\Delta_fH°(KF, cr) = -135.9 \pm 0.1\ kcal\cdot mol^{-1}$;[7] $\Delta_fH°(BF_3, g) = -271.42 \pm 0.4\ kcal\cdot mol^{-1}$,[7] we derive $\Delta_fH°(KBF_4, cr) = -450.5 \pm 0.7\ kcal\cdot mol^{-1}$ An average value, $\Delta_fH°(KBF_4, cr) = -451.0 \pm 1\ kcal\cdot mol^{-1}$, of these two results is adopted here.

Heat Capacity and Entropy

The heat capacity data are calculated from the high temperature enthalpy data of Dworkin and Bredig.[8] $S°(298.15\ K)$ is chosen such that a 3rd law analysis of the equilibrium data for the reaction $KBF_4(cr, l) = KF(cr, l) + BF_3(g)$ reported by de Boer and van Liempt[9] gives the experimentally determined heat of reaction at 25°C.[6]

Transition Data

T_{trs} is from the high temperature studies of Dworkin and Bredig.[8] $\Delta_{trs}H°$ is calcualted from their high temperature enthalpy data.

Fusion Data

T_{fus} has been reported as 803 K by de Boer and van Liempt[9] and 843 K by Dworkin and Bredig.[8] Dworkin and Bredig's value is adopted here. $\Delta_{fus}H°$ is calculated from their high temperature enthalpy data.

Sublimation Data

$\Delta_{sub}H°(298.15\ K)$ is estimated by comparison with data for $LiALF_4(cr)$ reported by Hildenbrand and Theard.[10]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200							
250							
298.15	114 483	133.888	133.888	0.	−1886.984	−1784.958	312.717
300	114 780	134.597	133.890	0.212	−1886.963	−1784.325	310.679
400	130.817	169.809	138.583	12.490	−1887.964	−1749.854	228.507
500	146.963	200.734	147.976	26.379	−1885.646	−1715.571	179.224
556.000	156.027	216.808	154.105	34.863	I <−−> II		
556.000	140.146	242.093	154.105	48.921	TRANSITION		
600	142.097	252.840	160.956	55.130	−1868.862	−1682.950	146.514
700	146.519	275.076	175.703	69.561	−1866.685	−1652.134	123.284
800	150.938	294.930	189.387	84.434	−1864.291	−1621.644	105.882
843.000	152.838	302.881	194.975	90.965	−−−−− II <−−> LIQUID −−−−−		
900	155.356	312.963	202.131	99.749	−1861.649	−1591.469	92.366
1000	159.779	329.560	214.054	115.505	−1858.748	−1561.602	81.570
1100	164.197	344.996	225.264	131.704	−1934.537	−1527.429	72.532
1200	168.619	359.472	235.851	148.345	−1930.056	−1490 614	64.885
1300	173.038	373.143	245.891	165.428	−1925.232	−1454 187	58.430
1400	177.456	386.129	255.448	182.953	−1920.057	−1418.145	52.912
1500	181.878	398.523	264.576	200.919	−1914.526	−1382.485	48.142

PREVIOUS: March 1965 CURRENT December 1969

Potassium Tetrafluoroborate (KBF_4) $B_1F_4K_1(cr)$

Potassium Tetraflouroborate (KBF_4) LIQUID $M_r = 125.901912$

$S°(298.15\ K) = [150.129]\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{fus} = 843\ K$

$\Delta_f H°(0\ K) = \text{Unknown}$
$\Delta_f H°(298.15\ K) = [-1869.415]\ kJ \cdot mol^{-1}$
$\Delta_{fus} H° = 17.66 \pm 0.16\ kJ \cdot mol^{-1}$

Enthalpy of Formation

$\Delta_f H°$(l, 298.15 K) is calculated from $\Delta_f H°$(cr) by adding $\Delta_{fus} H°$ and the difference in enthalpy, $H°(843\ K) - H°(298\ 15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The heat capacity data are calculated from the high temperature enthalpy data of Dworkin and Bredig.[1] $S°(298.15\ K)$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

T_{fus} has been reported as 803 K by de Boer and van Liempt[2] and 843 K by Dworkin and Bredig.[1] Dworkin and Bredig's value is adopted here. $\Delta_{fus} H°$ is calculated from their high temperature enthalpy data.

References

[1] A. S. Dworkin and M. A. Bredig, Oak Ridge Natl. Lab., personal communication, (September 23, 1969).
[2] J. H. de Boer and J. A. M. van Liempt, Rec. Trav. Chim. 46, 124 (1927).

Potassium Tetrafluoroborate (KBF_4) $B_1F_4K_1(l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

		$J \cdot K^{-1} mol^{-1}$		$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G° - H°(T_r)]/T$	$H° - H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0							
100							
200							
250							
298.15	167.117	150.129	150.129	0.	−1869.415	−1772.232	310.488
300	167.117	151 163	150.133	0.309	−1869.298	−1771.630	308.468
400	167.117	199.240	156.688	17.021	−1865 865	−1739.527	227 159
500	167.117	236.531	169.066	33 733	−1860 724	−1708.547	178.491
600	167.117	267.000	182.926	50 444	−1855.979	−1678.563	146.132
700	167 117	292.761	196.824	67.156	−1851.522	−1649.350	123.076
800	167 117	315 077	210.242	83.868	−1847.289	−1620.759	105.825
843.000	167.117	323.826	215.814	91.054	- - - - - II <- - > LIQUID - - - - -		
900	167.117	334.760	223.005	100.580	−1843.250	−1592.688	92.437
1000	167 117	352.368	235 077	117.291	−1839.393	−1565.056	81.750
1100	167 117	368.296	246.475	134.003	−1914.670	−1533.192	72.805
1200	167 117	382.837	257.241	150.715	−1910.118	−1498.713	65.237
1300	167.117	396.213	267.424	167.426	−1905.665	−1464.611	58 849
1400	167.117	408.598	277.071	184.138	−1901.303	−1430.848	53.386
1500	167.117	420.128	286.228	200.850	−1897.026	−1397.394	48.662

PREVIOUS: CURRENT: December 1969

Potassium Tetrafluoroborate (KBF_4) $B_1F_4K_1(l)$

Potassium Tetrafluoroborate (KBF_4) CRYSTAL(I–II)-LIQUID

0	to	556 K	crystal, I
556	to	843 K	crystal, II
above		843 K	liquid

Refer to the individual tables for details.

$M_r = 125.901912$ Potassium Tetrafluoroborate (KBF_4) $B_1F_4K_1(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = p° = 0.1 MPa

T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
0							
100							
200							
250							
298.15	114.483	133.888	133.888	0.	−1886.984	−1784.958	312.717
300	114.780	134.597	133.890	0.212	−1886.963	−1784.325	310.679
400	130.817	169.809	138.583	12.490	−1887.964	−1749.854	228.507
500	146.963	200.734	147.976	26.379	−1885.646	−1715.571	179.224
556.000	156.027	216.808	154.105	34.863		I <--> II	
556.000	140.146	242.093	154.105	48.921		TRANSITION	
600	142.097	252.840	160.956	55 130	−1868.862	−1682.950	146.514
700	146.519	275.076	175.703	69.561	−1866.685	−1652.134	123.284
800	150.938	294.930	189.387	84.434	−1864.291	−1621.644	105.882
843.000	152.838	302.881	194.975	90.965		II <--> LIQUID	
843.000	167.117	323.826	194.975	108.622		TRANSITION	
900	167.117	334.760	203.485	118.147	−1843.251	−1592.688	92.437
1000	167.117	352.368	217.509	134.859	−1839.394	−1565.057	81.750
1100	167.117	368.296	230.504	151.571	−1914.671	−1533.192	72.805
1200	167.117	382.837	242.601	168.283	−1910.118	−1498.714	65.237
1300	167.117	396.213	253.910	184.994	−1905.665	−1464.612	58.849
1400	167.117	408.598	264.522	201.706	−1901.304	−1430.849	53.386
1500	167.117	420.128	274.516	218.418	−1897.027	−1397.394	48.662

PREVIOUS: CURRENT: December 1969

Potassium Tetrafluoroborate (KBF_4) IDEAL GAS $M_r = 125.901912$ Potassium Tetrafluoroborate (KBF_4) $B_1F_4K_1(g)$

$\Delta_f H°(0\ K) = [1543.9 \pm 5]\ kJ \cdot mol^{-1}$

S(298.15 K) = [315.4 ± 3] J·K^{-1}·mol^{-1} $\Delta_f H°(298.15\ K) = [-1552.3 \pm 5]\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
[900](1)	[1000](1)	[300](2)
[450](1)	[300](1)	[500](2)
[350](1)	[250](1)	[1400](2)

Ground State Quantum Weight: [1] α = [3]
Point Group: [C_{3v}]
Bond Distances: B-F = 1.380 Å; K-F = 2.752 Å; B-K = [2.863] Å
Bond Angles: F-B-F = 109°28'; F_{ax}-B-K = [180]°
Product of Moments of Inertia: $I_A I_B I_C = [4.547923 \times 10^{-113}]\ g^3 \cdot cm^6$

Enthalpy of Formation

$\Delta_f H(g)$ is calculated from $\Delta_f H(cr)$ and the estimated enthalpy of sublimation.

Heat Capacity and Entropy

The vibrational frequencies are estimated by comparison with data for BF_4^-, BF_3, KF, and K_2F_2. The infrared and Raman spectra of BF_4^- in various phases have been reported by.[1-4] The molecular structure is assumed to be the same as for $LiAlF_4$ as discussed by Porter and Zeller.[5] The B–F and K–F bond lengths and F–B–F bond angle are average values of the crystallographic data recently reported by Clark and Lynton.[6] The B–K bond length is calcualted from the above structural data according to the assumed molecular model. The principal moments of inertia are $I_A = I_B = 16.0214 \times 10^{-39}$, and $I_B = I_C = 53.2791 \times 10^{-39}\ g \cdot cm^2$.

References

[1] G. L. Cote and H. W. Thompson, Proc. Royal Soc. (London), 210A, 217 (1951).
[2] J. O. Edwards, G C. Morrison, V. F. Ross, and J. W. Schultz, J. Amer. Chem. Soc. 77, 266 (1955).
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[4] J. A. A. Ketelaar and R. L. Fulton, Z. Elektrochem. 64, 641 (1960).
[5] R. F. Porter and E. E. Zeller, J. Chem. Phys. 33, 858 (1960).
[6] M. J. R. Clark and H. Lynton, Can. J. Chem. 47, 2579 (1969).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	S° (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	-17.598	-1543.916	-1543.916	INFINITE
100	45.326	242.588	382.561	-13.997	-1547.886	-1534.479	801.530
200	72.713	283.084	323.060	-7.995	-1550.669	-1519.843	396.942
250	81.920	300.343	316.820	-4.119	-1551.543	-1512.031	315.922
298.15	88.941	315.394	315.394	0.	-1552.264	-1504.354	263.557
300	89.184	315.944	315.395	0.165	-1552.291	-1504.057	261.880
350	95.129	330.153	316.504	4.777	-1555.374	-1495.865	223.246
400	100.093	343.189	319.036	9.661	-1556.073	-1487.315	194.223
450	104.277	355.227	322.397	14.774	-1556.687	-1478.683	171.641
500	107.817	366.402	326.245	20.078	-1557.226	-1469.986	153.568
600	113.376	386.578	334.657	31.153	-1558.120	-1452.450	126.447
700	117.425	404.375	343.370	42.703	-1558.823	-1434.781	107.065
800	120.418	420.260	352.007	54.603	-1559.403	-1417.020	92.522
900	122.668	434.579	360.399	66.762	-1559.916	-1399.191	81.207
1000	124.391	447.597	368.478	79.119	-1560.414	-1381.306	72.152
1100	125.731	459.518	376.220	91.628	-1639.894	-1358.760	64.522
1200	126.792	470.505	383.625	104.256	-1639.425	-1333.223	58.034
1300	127.643	480.689	390.705	116.979	-1638.961	-1307.725	52.545
1400	128.334	490.174	397.475	129.779	-1638.511	-1282.262	47.842
1500	128.903	499.049	403.954	142.642	-1638.083	-1256.831	43.767
1600	129.376	507.383	410.160	155.557	-1637.683	-1231.427	40.202
1700	129.774	515.239	416.113	168.515	-1637.314	-1206.048	37.057
1800	130.111	522.666	421.828	181.509	-1636.979	-1180.689	34.263
1900	130.399	529.709	427.322	194.535	-1636.677	-1155.348	31.763
2000	130.646	536.404	432.610	207.588	-1636.408	-1130.022	29.513
2100	130.861	542.784	437.706	220.663	-1636.171	-1104.709	27.478
2200	131.048	548.876	442.622	233.759	-1635.962	-1079.406	25.628
2300	131.212	554.705	447.369	246.872	-1635.777	-1054 112	23.940
2400	131.357	560.292	451.959	260.001	-1685.874	-1027.757	22.369
2500	131.485	565.657	456.400	273.143	-1685.808	-1000.337	20.901
2600	131.600	570.816	460.702	286.298	-1685.723	-972.920	19.546
2700	131.702	575.785	464.873	299.463	-1685.618	-945.506	18.292
2800	131.793	580.576	468.920	312.638	-1685.491	-918.097	17.127
2900	131.876	585.203	472.850	325.821	-1685.339	-890.692	16.043
3000	131 950	589.675	476.671	339.012	-1685.162	-863.294	15.031
3100	132.018	594.002	480.386	352.211	-1684.959	-835.902	14.085
3200	132.079	598.195	484.002	365.416	-1684.732	-808.516	13.198
3300	132.135	602.260	487.525	378.626	-1684.472	-781.139	12.364
3400	132.186	606.205	490.958	391.843	-1684.195	-753.769	11.580
3500	132.233	610.038	494.305	405.064	-1683.895	-726.408	10.841
3600	132.277	613.764	497.572	418.289	-1683.580	-699.056	10.143
3700	132.316	617.388	500.762	431.519	-1683.251	-671.712	9.483
3800	132.353	620.917	503.877	444.752	-1682.913	-644.379	8.858
3900	132.387	624.356	506.923	457.989	-1682.570	-617.053	8.264
4000	132.419	627.708	509.901	471.230	-1682.221	-589.737	7.701
4100	132.448	630.978	512.814	484.473	-1681.879	-562.430	7.165
4200	132.475	634.170	515.666	497.719	-2161 400	-528.105	6.568
4300	132.500	637.288	518.458	510.968	-2160.002	-489.235	5.943
4400	132.524	640.334	521.193	524.219	-2158.351	-450.422	5.347
4500	132.546	643.312	523.874	537.473	-2156.940	-411.621	4.778
4600	132.567	646.226	526.502	550.728	-2155.552	-372.852	4.234
4700	132.586	649.077	529.080	563.986	-2154.174	-334.114	3.713
4800	132.604	651.869	531.609	577.246	-2152.719	-295.418	3.215
4900	132.622	654.603	534 091	590.507	-2151.402	-256.738	2.737
5000	132.638	657.283	536.529	603.770	-2150.122	-218.084	2.278
5100	132.653	659.909	538.922	617.034	-2148.883	-179.456	1.838
5200	132.667	662.485	541.274	630.300	-2147.687	-140.851	1.415
5300	132.681	665.013	543.585	643.568	-2146.536	-102.269	1.008
5400	132.693	667.493	545.856	656.837	-2145.433	-63.709	0.616
5500	132.706	669.928	548.090	670.106	-2144.378	-25.168	0.239
5600	132.717	672.319	550.287	683.378	-2143.373	13.354	-0.125
5700	132.728	674.668	552.449	696.650	-2142.074	51.810	-0.475
5800	132.738	676.976	554.576	709.923	-2141.126	90.291	-0.813
5900	132.748	679.246	556.670	723.197	-2140.225	128.757	-1.140
6000	132.757	681.477	558.731	736.473	-2139.370	167.206	-1.456

PREVIOUS: December 1969 (1 atm) CURRENT December 1969 (1 bar)

S°(298.15 K) = [171.85] J·K^{-1}·mol^{-1}

$\Delta_f H^\circ$(0 K) = 439.5 ± 8.4 kJ·mol^{-1}
$\Delta_f H^\circ$(298.15 K) = 442.7 ± 8.4 kJ·mol^{-1}

Electronic Level and Quantum Weight State	ϵ_i, cm^{-1}	g_i
$^1\Sigma^+$	0	1

ω_e = [2368] cm^{-1} $\quad$ $\omega_e x_e$ = [49] cm^{-1} $\quad$ σ = 1
B_e = 12.036 cm^{-1} $\quad$ α_e = 0.413 cm^{-1} $\quad$ r_e = 1.2325 Å

Enthalpy of Formation

$\Delta_f H^\circ$(298.15 K) was calculated from D_0°(BH) = 3.39 ± 0.04 e.v. reported by Hurley.[1] Hurley stated "by combining an analysis of the spectroscopic data with theoretical calculations, we obtain a greatly improved estimate of D_0°(BH)" This value and the other D_0°(BH) values which are tabulated below are based on the same spectroscopic data but differ due to different methods of analysis.

D_0°(BH), eV	Method	Source
3.0 ± 0.4	Birge Sponer extrapolations	(2)
3.6	Observed predissociation by rotation in BH, A'Π and deduced D_0°(BH)	(3)
<3.51	Pre dissociation limit. This is only an upper limit due to a maximum in the potential curve of the A'Π state	(4)
3.38 ± 0.04	The potential energy curve of the A'Π state was determined and was found to have a maximum and a minimum in agreement with Herzberg and Mundie	The selected D_0°(BH) value as reported by Hurley (1).

Heat Capacity and Entropy

The molecular constants from Herzberg[4] were *adjusted for the natural abundance of* ^{10}B and ^{11}B. Because the constants ω_e and $\omega_e x_e$ could not be determined directly from the spectrum, Almy and Horsfall[3] obtained estimates for the ground state X $^1\Sigma^+$ from the rotational constants for this state and the relations $D_e = 4B_e^3/\omega_e^2$ and $\omega_e x_e/\omega_e = 0.6\ \alpha_e/B_e$.

References

[1] A. C. Hurley, Proc. Royal Soc. (London) **A261**, 237 (1961).
[2] A. G. Gaydon, "Dissociation Energies and Spectra of Diatomic Molecules," 2nd ed. Chapman and Hall, Ltd., London, 261 pp. (1953).
[3] G M. Almy and R. B. Horsfall, Jr., Phys. Rev. *51*, 491 (1937).
[4] G. Herzberg and L. G. Mundle, J. Chem. Phys. 8, 263 (1940) and G. Herzberg, "Spectra of Diatomic Molecules", D. Van Nostrand Co., Inc., York, (1950).

Enthalpy Reference Temperature = T_r = 298.15 K $\qquad$ Standard State Pressure = p° = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	S°	$-[G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−8.639	439.476	439.476	INFINITE
90	29.126	140.014	197.766	−5.775	440.816	431.882	−225.592
200	29.143	160.207	174.516	−2.862	442.050	422.433	−110.328
250	29.156	166.712	172.329	−1.404	442.438	417.481	−87.228
298.15	29.181	171.849	171.849	0.	442.667	412.651	−72.295
300	29.182	172.029	171.849	0.054	442.673	412.465	−71.816
350	29.240	176.532	172.205	1.514	442.782	407.420	−60.804
400	29.347	180.442	172.995	2.979	442.783	402.367	−52.544
450	29.514	183.908	174.019	4.450	442.696	397.319	−46.120
500	29.741	187.029	175.166	5.931	442.543	392.285	−40.982
600	30.340	192.502	177.612	8.934	442.100	382.272	−33.280
700	31.052	197.231	180.084	12.003	441.545	372.344	−27.785
800	31.792	201.426	182.495	15.145	440.928	362.500	−23.669
900	32.503	205.212	184.812	18.360	440.274	352.735	−20.472
1000	33.160	208.671	187.027	21.644	439.594	343.045	−17.919
1100	33.752	211.860	189.142	24.990	438.890	333.424	−15.833
1200	34.280	214.820	191.160	28.392	438.164	323.868	−14.098
1300	34.748	217.583	193.087	31.844	437.414	314.373	−12.632
1400	35.162	220.173	194.930	35.340	436.639	304.938	−11.377
1500	35.530	222.612	196.695	38.875	435.835	295.558	−10.292
1600	35.859	224.916	198.388	42.445	435.003	286.233	−9.345
1700	36.152	227.099	200.013	46.046	434.141	276.961	−8.510
1800	36.417	229.173	201.576	49.674	433.248	267.741	−7.770
1900	36.657	231.148	203.081	53.328	432.324	258.571	−7.109
2000	36.875	233.034	204.531	57.005	431.368	249.451	−6.515
2100	37.075	234.838	205.932	60.703	430.381	240.379	−5.979
2200	37.259	236.567	207.285	64.419	429.361	231.356	−5.493
2300	37.429	238.227	208.595	68.154	428.309	222.379	−5.050
2400	37.587	239.823	209.863	71.905	376.966	214.517	−4.669
2500	37.736	241.361	211.092	75.671	375.772	207.773	−4.341
2600	37.875	242.844	212.285	79.452	374.579	201.077	−4.040
2700	38.007	244.275	213.444	83.246	373.386	194.426	−3.761
2800	38.132	245.660	214.570	87.053	372.193	187.820	−3.504
2900	38.250	247.000	215.665	90.872	371.001	181.256	−3.265
3000	38.364	248.299	216.731	94.703	369.808	174.733	−3.042
3100	38.472	249.559	217.770	98.544	368.615	168.251	−2.835
3200	38.577	250.782	218.783	102.397	367.421	161.806	−2.641
3300	38.677	251.970	219.770	106.260	366.227	155.399	−2.460
3400	38.775	253.126	220.734	110.132	365.033	149.028	−2.290
3500	38.869	254.252	221.676	114.015	363.837	142.693	−2.130
3600	38.961	255.348	222.596	117.906	362.641	136.391	−1.979
3700	39.050	256.417	223.496	121.807	361.445	130.123	−1.837
3800	39.137	257.459	224.376	125.716	360.247	123.887	−1.703
3900	39.222	258.477	225.237	129.634	359.048	117.683	−1.576
4000	39.305	259.471	226.081	133.560	357.848	111.509	−1.456
4100	39.386	260.443	226.907	137.495	356.648	105.366	−1.342
4200	39.467	261.393	227.717	141.437	−124.404	106.276	−1.322
4300	39.545	262.322	228.511	145.388	−124.520	111.769	−1.358
4400	39.623	263.232	229.290	149.346	−124.639	117.266	−1.392
4500	39.699	264.123	230.054	153.313	−124.761	122.765	−1.425
4600	39.774	264.997	230.804	157.286	−124.886	128.267	−1.457
4700	39.848	265.853	231.541	161.267	−125.015	133.771	−1.487
4800	39.922	266.693	232.264	165.256	−125.148	139.279	−1.516
4900	39.994	267.517	232.975	169.252	−125.285	144.789	−1.543
5000	40.066	268.325	233.674	173.255	−125.425	150.303	−1.570
5100	40.137	269.119	234.362	177.265	−125.570	155.818	−1.596
5200	40.207	269.900	235.038	181.282	−125.719	161.337	−1.621
5300	40.277	270.666	235.703	185.306	−125.872	166.859	−1.644
5400	40.346	271.420	236.357	189.337	−126.030	172.384	−1.667
5500	40.415	272.161	237.001	193.375	−126.192	177.911	−1.690
5600	40.483	272.889	237.636	197.420	−126.358	183.442	−1.711
5700	40.551	273.606	238.261	201.472	−126.529	188.976	−1.732
5800	40.618	274.312	238.876	205.530	−126.704	194.513	−1.752
5900	40.685	275.007	239.483	209.596	−126.884	200.052	−1.771
6000	40.752	275.692	240.080	213.667	−127.068	205.595	−1.790

PREVIOUS: December 1964 (1 atm) $\qquad$ CURRENT: December 1964 (1 bar)

Boron Hydride Oxide (HBO) **IDEAL GAS** $M_r = 27.81734$ **Boron Hydride Oxide (HBO)** $B_1H_1O_1(g)$

$S°(298.15 \text{ K}) = [202.6 \pm 0.5] \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_fH°(0 \text{ K}) = -197.7 \pm 3.0 \text{ kJ·mol}^{-1}$

$\Delta_fH°(298.15 \text{ K}) = -198.3 \pm 3.0 \text{·kJ·mol}^{-1}$

Electronic Levels and Quantum Weights

ϵ_i, cm^{-1}	g_i	ϵ_i, cm^{-1}	g_i
0	[1]	[35000]	[6]
[30000]	[3]	[40000]	[3]

Vibrational Frequencies and Degeneracies

υ, cm^{-1}
[2802](1)
757 (2)
1822 (1)

Ground State Configuration: $[^1\Sigma^+]$ $\sigma = 1$

Point Group: $C_{\infty v}$

Bond Distances: H–B = [1.17] Å; H–O = [1.19] Å

Bond Angle: H–B–O = [180°]

Rotational Constant· $B_0 = [1.341144]$ cm^{-1}

Enthalpy of Formation

We calculate $\Delta_fH°$ from a selected value, $\Delta_fH°(\text{DBO, g}) = -47.95$ kcal·mol^{-1}, by combining this value with zero–point energies and relative enthalpies, $H°(298.15 \text{ K})–E_0°$, for HBO, D_2, DBO and H_2. All ancillary data are from JANAF[1] unless otherwise indicated. The zero–point energies are estimated as one–half the sum of the vibrational frequencies. The vibrational frequencies for DBO are taken from the matrix–isolation results of Lory and Porter.[2] We assume that DBO and HBO have similar structures, and we calculate the relative enthalpy for DBO as $H°(298.15 \text{ K}) -E_0° = -2.27$ kcal·mol^{-1}. Data for D_2 are taken from NBS.[3]

The selected value of $\Delta_fH°$ for DBO is obtained from the results of a mass–spectrometric study[4, 5] of the reaction of D (g) with $B_2O_3(l)$. The thermal results which were initially reported[4] for a study of the reactions (A) $D_2(g) + B_2O_3(l) = DBO(g) + DOBO(g)$ and (B) $D_2O(g) + B_2O_3(l) = 2DOBO(g)$ are unreliable due to erroneous equilibrium constants. 2nd–law enthalpies for these two reactions have been reported in revised form in a later publication.[5] Apparently, no attempt was made in this study to perform calibration experiments which would have allowed the ion intensity data to be converted to absolute partial pressures; thus, precluding a 3rd law analysis. We combine their 2nd law values[5] for Δ_rH (1296 K) for reactions (A) and (B) to give $\Delta_rH(1296 \text{ K}) = 135 \pm 4$ kcal·mol^{-1} for the process $2D_2(g) + B_2O_3(l) = 2DBO(g) + D_2O(g)$. Corrected to 298.15 K this value is 144.1 kcal·mol^{-1} which leads to $\Delta_fH°(\text{DBO,g, 298.15 K}) = -47.95 \pm 2.3$ kcal·mol^{-1} with $\Delta_fH°(D_2O, \text{ g, 298.15 K}) = -59.561 \pm 0.02$ kcal·mol^{-1}[13] and $\Delta_fH°(B_2O_3, \text{ l, 298.15 K}) = 299.56 \pm 0.6$ kcal·mol^{-1}.[1]

Comparison of values for the stretching force constants in HBO, BH_3,[6] BO, and B_2O_2[1] suggests a similarity in the bonds of these molecules. Using $D_0°(298.15 \text{ K})$ (H–B) = $\bar{D}°(298.15 \text{ K})$ (BH_3) = 87.9 kcal·mol^{-1} and $D_0°(298.15 \text{ K})$ (B=O) = $D_0°(298.15 \text{ K})$ (BO) + $D_0°(298.15 \text{ K})$ (B_2O_2) /2 = 202 kcal·mol^{-1},[1] we calculate an enthalpy of atomization for HBO of 298.9 kcal·mol. This corresponds to $\Delta_fH°(\text{HBO, g, 298.15 K}) = -45.4$ kcal·mol^{-1} which lends support to the experimental measurements at Farber *et al.*[4 5] Pervious JANAF estimates[7] of $\Delta_fH°$ via bond energy calculations led to results which were too positive due to the use of an inaccurate value (168 kcal·mol^{-1}) for $D_0°$ (B=O). A recent ab–initio LCAO–MO–SCF investigation[8] of HBO yields $\Delta_{at}H = 232.2$ kcal·mol^{-1}; however, this value does not include a contribution from correlation effects[9, 16] and therefore is too low.

Heat Capacity and Entropy

The B=O stretching $(\upsilon)_3$ and bending $(\upsilon)_2$ frequencies for the isotopes $H^{11}BO$ and $H^{10}BO$ have been measured in a low–temperature argon matrix.[2] These values are corrected for the natural isotopic abundances of boron. The H–B stretching frequency $(\upsilon)_1$ is calculated from an estimated force constant by the valence force method.[10] The stretching force constant K_1 is estimated from the ratio $K_1/K_D/l_1l_2 = 17.47$ which is the value we calculate for DBO from the measured frequencies of Lory and Porter.[2] These workers[2] used a slightly different value for K_1 and obtained a value for υ_1 which is roughly 50 cm^{-1} higher than our result. We believe our estimate is probably more nearly correct, since it agrees much better with the H–B stretching frequency (2808 cm^{-1}) observed for BH_3.[6] MO calculations show that the pattern of valence orbitals for HBO is similar to that in HCN[8] and HCP.[11 16] The ordering is substantiated by the photoelectron spectra[12] which have been observed for HCN and HCP. This suggests that the ground and excited electronic states for these isoelectronic molecules are quite similar. We assume that the ground state configuration is $^1\Sigma^+$ by analogy with those for HCN and HCP.[1] We also include three triplet levels which are estimated from those observed for HCP[1] and predicted for HCN.[13]

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−9.156	−197.688	−197.688	INFINITE
100	29.137	168.766	231.276	−6.251	−197.759	−200.903	104 941
200	31.249	189.398	205.712	−3.263	−197.906	−204.013	53.283
250	33.279	196.585	203.187	−1.650	−198.092	−205.519	42.941
298.15	35.260	202.617	202.617	0.	−198.322	−206.929	36.253
300	35.334	202.836	202.618	0.065	−198.331	−206.983	36.039
350	37.224	208.427	203.055	1.880	−198.606	−208.403	31.102
400	38.923	213.510	204.049	3.785	−198.913	−209.782	27.395
450	40.455	218.185	205.363	5.770	−199.244	−211.121	24.506
500	41.853	222.521	206.865	7.828	−199.591	−212.422	22.192
600	44.343	230.377	210.142	12.141	−200.304	−214.921	18.711
700	46.511	237.379	213.542	16.686	−201.010	−217.302	16.215
800	48.408	243.716	216.924	21.434	−201.690	−219.582	14.337
900	50.061	249.516	220.228	26.359	−202.336	−221.779	12.872
1000	51.495	254.866	223.427	31.439	−202.952	−223.907	11.696
1100	52.734	259.834	226.514	36.652	−203.543	−225.973	10.731
1200	53.802	264.469	229.486	41.980	−204.117	−227.987	9.924
1300	54.724	268.813	232.346	47.407	−204.683	−229.953	9.240
1400	55.520	272.898	235.098	52.920	−205.249	−231.876	8.651
1500	56.208	276.753	237.748	58.508	−205.820	−233.758	8.140
1600	56.806	280.400	240.300	64.159	−206.404	−235.601	7.692
1700	57.327	283.860	242.762	69.866	−207.006	−237.408	7.295
1800	57.783	287.150	245.137	75.622	−207.629	−239.178	6.941
1900	58.182	290.285	247.431	81.421	−208.278	−240.914	6.623
2000	58.534	293.278	249.650	87.257	−208.956	−242.614	6.336
2100	58.846	296.142	251.796	93.126	−209.665	−244.279	6.076
2200	59.122	298.886	253.874	99.025	−210.407	−245.910	5.839
2300	59.369	301.519	255.889	104.950	−211.183	−247.507	5.621
2400	59.589	304.051	257.843	110.898	−262.256	−248.000	5.398
2500	59.786	306.487	259.741	116.867	−263.184	−247.387	5.169
2600	59.964	308.836	261.584	122.855	−264.119	−246.737	4.957
2700	60.125	311.102	263.376	128.859	−265.060	−246.050	4.760
2800	60.271	313.291	265.120	134.879	−266.008	−245.329	4.577
2900	60.404	315.409	266.818	140.913	−266.965	−244.574	4.405
3000	60.525	317.458	268.472	146.960	−267.931	−243.785	4.245
3100	60.636	319.445	270.084	153.018	−268.906	−242.964	4.094
3200	60.739	321.372	271.657	159.087	−269.890	−242.112	3.952
3300	60.835	323.242	273.192	165.165	−270.883	−241.228	3.818
3400	60.924	325.060	274.691	171.253	−271.886	−240.314	3.692
3500	61.008	326.827	276.155	177.350	−272.899	−239.371	3.572
3600	61.088	328.547	277.587	183.455	−273.921	−238.399	3.459
3700	61.165	330.221	278.987	189.567	−274.953	−237.398	3.351
3800	61.239	331.854	280.357	195.688	−275.994	−236.369	3.249
3900	61.312	333.445	281.698	201.815	−277.044	−235.312	3.152
4000	61.385	334.998	283.011	207.950	−278.103	−234.229	3.059
4100	61.457	336.515	284.297	214.092	−279.171	−233.119	2.970
4200	61.531	337.997	285.558	220.242	−760.096	−224.959	2.798
4300	61.606	339.446	286.795	226.398	−760.092	−212.217	2.578
4400	61.684	340.863	288.008	232.563	−760.098	−199.476	2.368
4500	61.766	342.250	289.198	238.735	−760.113	−186.735	2.168
4600	61.851	343.608	290.366	244.916	−760.136	−173.993	1.976
4700	61.941	344.940	291.513	251.106	−760.168	−161.250	1.792
4800	62.036	346.245	292.640	257.305	−760.208	−148.507	1.616
4900	62.138	347.525	293.747	263.513	−760.256	−135.762	1.447
5000	62.246	348.781	294.835	269.732	−760.311	−123.017	1.285
5100	62.361	350.015	295.905	275.963	−760.372	−110.270	1.129
5200	62.483	351.227	296.957	282.205	−760.441	−97.523	0.980
5300	62.614	352.419	297.992	288.460	−760.515	−84.773	0.835
5400	62.753	353.590	299 011	294.728	−760.595	−72.023	0.697
5500	62.901	354.743	300.014	301.010	−760.679	−59.271	0.563
5600	63.058	355.878	301.001	307.308	−760.768	−46.517	0.434
5700	63.225	356.995	301.974	313.622	−760.861	−33.762	0.309
5800	63.401	358.096	302.932	319.954	−760.957	−21.005	0.189
5900	63.587	359.182	303.876	326.303	−761.056	−8.247	0.073
6000	63 783	360.252	304.807	332.671	−761.158	4.514	−0.039

PREVIOUS. December 1975 (1 atm) CURRENT: December 1975 (1 bar)

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Boron Hydride Oxide, Ion (HBO$^+$)   IDEAL GAS M_r = 27.81679   Boron Hydride Oxide, Ion (HBO$^+$) $B_1H_1O_1^+(g)$

$S°(298.15\ K) = [214.57 \pm 6.3]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [1182.0 \pm 12]\ kJ{\cdot}mol^{-1}$

$\Delta_fH°(298.15\ K) = [1187.5 \pm 12]\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ε, cm^{-1}	g_i
$X^2\Pi$	0	[4]
$A^2\Sigma^+$	[6000]	[2]
$B^2\Sigma^+$	[40000]	[2]

Vibrational Frequencies and Degeneracies

ν, cm^{-1}
[2559](1)
[801](2)
[1617](1)

Point Group: [$C_{\infty v}$]   σ = 1

Bond Distances: H–B = [1.19] Å;   B–O = [1.25] Å

Bond Angle: H–B–O = [180]°

Rotational Constant. B_0 = [1.228629] cm^{-1}

Enthalpy of Formation

The HBO$^+$ ion has been detected mass spectrometrically by Sholette and Porter[1] and Farber and Frisch.[2] However, no appearance potential data have been reported for the ion. Kroto *et al.*[3] recently attempted to measure the photelectron spectrum of HBO by passing water vapor over heated boron. The spectrum showed no bands which could be definitely assigned to HBO monomer. Unfortunately, the region of their spectrum (~14–15 eV) where the first photoelectron band of HBO would be expected to lie shows a broad band which also appeared in the spectrum of HBS above 1150°C. Kroto *et al.*[4] have assigned this band to diborane. We believe the HBO band may well be hidden under this broad band.

We employ Koopmans' theorem[4] to obtain the ionization potential of HBO as 14.3 eV from the one electron orbital energies reported by Thomson and Wishart.[5] A comparison of Koopmans' theorem IP's for the related species HBS,[6] HCN,[5] and HCP[7] with experimental values[8,9] shows that the theoretical calculations correctly predict these ionization potentials to within about ± 0.4 eV. We adopt $\Delta_rH° = 329.7_6 \pm 9$ kcal·mol^{-1} for the ionization process $HBO(g) + e^- = HBO^+(g) + 2e^-$ at 0 K, and we obtain $\Delta_fH°(HBO^+, g, 0\ K) = 282.6 \pm 12.0$ kcal·mol^{-1} when the former value is combined with $\Delta_fH°(HBO, g, 0\ K) = -47.2 \pm 3.0$ kcal·mol^{-1}[18]. $\Delta_fH°(298.15\ K)$ is 283.8 ± 12.0 kcal·mol^{-1}.

Heat Capacity and Entropy

Extensive ab initio MO calculations[5] reported for HBO show that the highest occupied orbital is of Π–symmetry and is localized mainly on the oxygen atom. The Walsh diagram[10] for HAB molecules predicts that this orbital is bonding. We would expect therefore that the ion is less strongly bound than the parent molecule. For HCN which has the same orbital ordering as HBO,[5] ionization[11] occurs with a 2.2% increase in the H–C bond length and a 4.7% increase in the C=N bond length. We assume a similar increase in the bond lengths of HBO[8] upon loss of the bonding electron. A linear configuration is assumed by analogy with that for HBS$^+$.[8] This assumption is supported by predictions from the Walsh diagram.[10]

All vibrational frequencies are calculated from estimated force constants by a valence force method.[12] The force constants are estimated from those for HBO[8] by comparison with the changes in the changes in the force constants for HCN[8] produced on ionization.[9] The electronic states and levels are estimated from those observed for isoelectronic ions HBS$^+$, and HCP$^+$.[9] We estimate the uncertainties in our calculated frequencies as ±50 cm^{-1} which introduces an error of only about ±0.1 cal·K^{-1}·mol^{-1} in the value of S°(298 15 K). The uncertainty in the electronic levels contribute the majority of the error in the entropy. We predict that the energy separation of the $^2\Pi$–$^2\Sigma$ states is small. Thus, it is possible that the ground state is $^2\Sigma$ as is the case for the isoelectronic ions CO$^+$ and N_2^+.[13] If the ground state is $^2\Sigma$, then our entropies should be decreased by roughly 1.5 gibbs/mol at all temperatures above 298.15 K. The enthalpy is much more certain than the entropy. Below 2000 K the uncertainty in our relative enthalpies probably does not exceed a few calories. The uncertainty increases at higher temperatures and is about 1.0 kcal·mol^{-1} at 4000 K. All excited states are expected to be linear as observed for HBS$^+$.[3]

References

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_fH°$ (kJ·mol^{-1})	$\Delta_fG°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	−9.090	1182.047		
90	29.122	181.019	242.861	−6.184			
200	30.857	201.543	217.612	−3.214			
250	32.755	208.626	215.126	−1.625			
298.15	34.744	214.565	214.565	0.	1187.545	1169.120	−204.825
300	34.821	214.780	214.566	0.064	1187.573	1169.006	−203.542
350	36.828	220.300	214.997	1.856	1188.314	1165.852	−173.994
400	38.701	225.342	215.979	3.745	1189.031	1162.594	−151.819
450	40.425	230.001	217.282	5.724	1189.732	1159.248	−134.562
500	42.011	234.343	218.773	7.785	1190.428	1155.823	−120.748
600	44.817	242.258	222.041	12.130	1191.826	1148.771	−90.009
700	47.203	249.351	225.444	16.734	1193.258	1141.483	−85.178
800	49.235	255.790	228.841	21.559	1194.733	1133.986	−74.042
900	50.965	261.692	232.168	26.571	1196.252	1126.302	−65.369
1000	52.442	267.140	235.396	31.744	1197.808	1118.447	−58.422
1100	53.711	272.199	238.515	37.053	1199.392	1110.434	−52.730
1200	54.808	276.921	241.520	42.480	1200.995	1102.276	−47.981
1300	55.765	281.346	244.416	48.010	1202.610	1093.984	−43.957
1400	56.606	285.510	247.204	53.629	1204.230	1085.568	−40.503
1500	57.350	289.442	249.890	59.328	1205.848	1077.035	−37.506
1600	58.012	293.164	252.479	65.096	1207.460	1068.395	−34.880
1700	58.605	296.699	254.977	70.928	1209.061	1059.655	−32.559
1800	59.138	300.065	257.389	76.816	1210.648	1050.820	−30.494
1900	59.618	303.275	259.720	82.754	1212.217	1041.898	−28.644
2000	60.050	306.344	261.975	88.738	1213.765	1032.894	−26.976
2100	60.441	309.284	264.159	94.762	1215.291	1023.813	−25.466
2200	60.794	312.104	266.274	100.824	1216.791	1014.660	−24.091
2300	61.112	314.813	268.326	106.920	1218.263	1005.439	−22.834
2400	61.400	317.420	270.318	113.046	1169.447	997.223	−21.704
2500	61.659	319.932	272.253	119.199	1170.782	990.020	−20.685
2600	61.893	322.355	274.133	125.377	1172.116	982.763	−19.744
2700	62.103	324.695	275.963	131.577	1173.449	975.455	−18.871
2800	62.292	326.957	277.744	137.797	1174.779	968.097	−18.060
2900	62.462	329.146	279.479	144.035	1176.105	960.692	−17.304
3000	62.614	331.266	281.170	150.289	1177.425	953.242	−16.597
3100	62.749	333.321	282.819	156.557	1178.739	945 747	−15.936
3200	62.870	335.316	284.429	162.838	1180.046	938.210	−15.315
3300	62.978	337.252	286.000	169.130	1181.345	930.633	−14.731
3400	63.074	339.133	287.535	175.433	1182.635	923.016	−14.180
3500	63.159	340.963	289.036	181.745	1183.916	915.362	−13.661
3600	63.233	342.743	290.503	188.065	1185.187	907.671	−13.170
3700	63.299	344.477	291.939	194.391	1186.448	899.944	−12.705
3800	63.356	346.166	293.344	200.724	1187.698	892.185	−12.264
3900	63.407	347.812	294.719	207.062	1188.938	884.392	−11.845
4000	63.450	349.418	296.067	213.405	1190.165	876.567	−11.447
4100	63.487	350.985	297.387	219.752	1191.381	868.712	−11.068
4200	63.519	352.515	298.681	226.102	712.735	867.852	−10.793
4300	63.546	354.010	299.951	232.456	715.014	871.518	−10.587
4400	63.569	355 472	301.196	238.812	717.278	875.131	−10.389
4500	63.588	356.900	302.418	245.169	719.527	878.693	−10.200
4600	63.603	358.298	303.618	251.529	721.761	882.206	−10.018
4700	63.615	359.666	304.796	257.890	723.979	885.670	−9.843
4800	63.624	361.005	305.953	264.252	726.181	889 087	−9.675
4900	63.630	362.317	307.090	270.614	728.366	892.458	−9.514
5000	63.635	363.603	308.207	276.978	730.534	895.785	−9.358
5100	63.637	364.863	309.306	283.341	732.684	899.069	−9.208
5200	63 638	366.099	310.386	289.705	734.816	902.310	−9.064
5300	63.637	367.311	311.449	296.069	736.929	905.511	−8.924
5400	63.634	368.500	312.495	302.432	739.023	908.672	−8.790
5500	63.631	369.668	313.523	308.796	741.098	911.794	−8.659
5600	63.627	370.815	314.536	315.158	743.153	914.880	−8.534
5700	63 621	371.941	315.534	321.521	745.187	917.928	−8.412
5800	63.615	373.047	316.516	327.883	747.200	920.942	−8.294
5900	63.609	374 135	317.483	334.244	749.191	923 919	−8.180
6000	63 602	375.204	318 436	340.604	751.160	926.864	−8.069

PREVIOUS: December 1975 (1 atm)   CURRENT. December 1975 (1 bar)

Boron Hydride Oxide, Ion (HBO^-) IDEAL GAS $M_r = 27.81789$ Boron Hydride Oxide, Ion (HBO^-) $B_1H_1O_1^-(g)$

$S°(298.15\ K) = [227.1 \pm 2.0]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [-238.5 \pm 24]\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = [-244.5 \pm 24]\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights ϵ, cm^{-1}	g_i
0	[2]
[10000]	[2]

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[2000] (1)
[1000] (1)
[1500] (1)

Ground State Quantum Weight: [2] $\sigma = 1$
Point Group: C_s
Bond Distances: H–B = [1.25] Å; B–O = [1.37] Å
Bond Angle: H–B–O = 123°
Product of Moments of Inertia: $I_AI_BI_C = [9.09027 \times 10^{-118}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The identification of the HBO^- radical has been made from observations of its electron spin resonance spectra which was measured[1 2] in γ–irradiated polycrystalline potassium borohydride. This assignment is confirmed by the fact that hyperfine coupling constants calculated by INDO[3] and UHF[4,5] methods are in reasonable agreement with the spectral data.[2] No experimental measurement of the electron affinity (EA) has been reported: however, recent MO calculations[6] predict that the value is small. We note that these calculations predict incorrectly the relative stabilities of HBO and HBO^- and therefore are of no use in the establishment of the absolute value of EA. This inversion in the predicted stabilities of the radical and parent molecule most likely arises from the neglect of correlation effects.

We estimate $\Delta_f H°$ from a consideration of bond–energy schemes. For the dissociative process $HBO^-(g) = H(g) + B(g) + O^-(g)$, we assume $\Delta_a H°(HBO,g,\ 0\ K) = 289.4\ kcal{\cdot}mol^{-1}$.[7] This atomization energy gives $\Delta_f H°(HBO^-,\ g,\ 0\ K) = -81.0\ kcal{\cdot}mol^{-1}$ which we believe is an upper limit since the unpaired electron in HBO^- is antibonding[8] and consequently, one would expect $\Delta_{at} H°(HBO^-) < \Delta_{at} H°(HBO)$. A lower limit of $\Delta_f H°$ can be obtained from a consideration of the H–B bond dissociation energy. It is very unlikely that $D_0^\circ(H\text{–}BO^-) < D_0^\circ(H\text{–}CO)$ which is equal to $14.1\ kcal{\cdot}mol^{-1}$. Using this value for $D_0^\circ(H\text{–}BO^-)$, we obtain $\Delta_f H°(HBO^-,\ g,\ 0\ K) = -33\ kcal{\cdot}mol^{-1}$ with $\Delta_f H°(H,g,\ 0\ K) = 52.103\ kcal{\cdot}mol^{-1}$ [7] and $\Delta_f H°(BO^-,\ g,\ 0\ K) = -71.0\ kcal{\cdot}mol^{-1}$.[9] We adopt an average ($-57 \pm 24\ kcal{\cdot}mol^{-1}$) of the upper and lower limit values. Our adopted $\Delta_f H°$ value corresponds to an $EA(HBO^-)$ of 0.42 ± 1.0 eV.

Heat Capacity and Entropy

The bond lengths are those reported by Thomson[3] who performed an INDO calculation in which the bond lengths were determined by minimization of the total energy. The esr spectrum[1 2] of HBO^- is consistent with a bent structure. Catton *et al.*[2] obtained bond angles of 121° and 125° from the p:s ratios deduced from estimated and observed anisotropic components of the hyperfine tensors. A similar calculation[2] for HCO and HCN^- led to bond angles which agreed with independent values to within ±5°. We adopt a bond angle of 123 ± 5°. MO calculations[3] give an angle of 129°. However, the energy minimization procedure with the INDO method generally over–estimates the angle as evidenced by the results for HCO[10] and HCN.[2 1] The principal moments of inertia are: $I_A = 0.1484 \times 10^{-39}$, $I_B = 2.4017 \times 10^{-39}$, and $I_C = 2.5501 \times 10^{-39}\ g{\cdot}cm^2$.

The electronic levels and quantum weights are taken from those for HCO,[7] which is isoelectronic with HBO^-. The vibrational frequencies arae estimated by comparison with the corresponding values for HBO, HBO^+, HCO and HCO^+.[7]

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[6] C. Thomson and B. J. Wishart, Theoret. Chim. Acta, 35, 267 (1974).
[7] JANAF Thermochemical Tables: HBO(g) and HBO (⁺g), 12-31-75; H(g), 6-30-74; B(g), 12-31-64; O (⁻g), 6-30-65; HCO(g) and HCO (g),⁺12-31-70.
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	C_p°	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.027	−238.827		
100	33.259	190.280	257.292	−6.701			
200	33.602	213.386	230.216	−3.366			
250	34.257	220.947	227.632	−1.671			
298.15	35.199	227.058	227.058	0.	−244.471	−254.111	44.519
300	35.240	227.276	227.058	0.065	−244.519	−254.171	44.255
350	36.456	232.797	227.492	1.857	−245.857	−255.674	38.157
400	37.806	237.752	228.470	3.713	−247.251	−256.982	33.558
450	39.211	242.286	229.756	5.638	−248.682	−258.113	29.961
500	40.609	246.490	231.222	7.634	−250.131	−259.083	27.066
600	43.240	254.131	234.416	11.829	−253.040	−260.600	22.687
700	45.531	260.973	237.729	16.270	−255.928	−261.632	19.523
800	47.454	267.182	241.029	20.923	−258.782	−262.251	17.123
900	49.042	272.866	244.255	25.750	−261.605	−262.515	15.236
1000	50.345	278.103	247.381	30.722	−264.407	−262.466	13.710
1100	51.417	282.953	250.397	35.811	−267.200	−262.136	12.448
1200	52.304	287.466	253.301	40.999	−269.994	−261.553	11.385
1300	53.044	291.683	256.093	46.267	−272.797	−260.736	10.476
1400	53.669	295.637	258.778	51.604	−275.618	−259.702	9.690
1500	54.205	299.359	261.360	56.998	−278.461	−258.467	9.001
1600	54.672	302.873	263.846	62.443	−281.331	−257.040	8.391
1700	55.085	306.200	266.240	67.931	−284.230	−255.433	7.849
1800	55.457	309.359	268.549	73.458	−287.161	−253.655	7.361
1900	55.798	312.367	270.777	79.021	−290.124	−251.713	6.920
2000	56.115	315.237	272.928	84.617	−293.120	−249.614	6.519
2100	56.413	317.982	275.009	90.244	−296.150	−247.364	6.153
2200	56.697	320.613	277.022	95.899	−299.214	−244.969	5.816
2300	56.968	323.139	278.973	101.583	−302.311	−242.435	5.506
2400	57.230	325.569	280.864	107.293	−355.700	−238.696	5.195
2500	57.484	327.911	282.699	113.028	−358.940	−233.754	4.884
2600	57.729	330.170	284.482	118.789	−362.180	−228.682	4.594
2700	57.968	332.353	286.215	124.574	−365.419	−223.486	4.324
2800	58.199	334.466	287.901	130.382	−368.658	−218.170	4.070
2900	58.423	336.512	289.542	136.213	−371.896	−212.739	3.832
3000	58.639	338.496	291.141	142.067	−375.134	−207.195	3.608
3100	58.848	340.422	292.699	147.941	−378.371	−201.544	3.396
3200	59.049	342.294	294.220	153.836	−381.608	−195.788	3.196
3300	59.242	344.114	295.705	159.751	−384.844	−189.931	3.006
3400	59.427	345.885	297.155	165.684	−388.080	−183.976	2.826
3500	59.603	347.610	298.572	171.636	−391.316	−177.926	2.655
3600	59.771	349.292	299.957	177.604	−394.553	−171.783	2.493
3700	59.930	350.932	301.313	183.590	−397.791	−165.551	2.337
3800	60.081	352.532	302.640	189.590	−401.030	−159.230	2.189
3900	60.223	354.095	303.939	195.605	−404.271	−152.825	2.047
4000	60.357	355.621	305.212	201.634	−407.515	−146.337	1.911
4100	60.482	357.113	306.460	207.676	−410.761	−139.767	1.781
4200	60.599	358.572	307.683	213.731	−893.860	−126.094	1.568
4300	60.707	359.999	308.884	219.796	−896.027	−107.788	1.309
4400	60.808	361.396	310.061	225.872	−898.200	−89.432	1.062
4500	60.902	362.763	311.217	231.957	−900.380	−71.026	0.824
4600	60.988	364.103	312.352	238.052	−902.568	−52.572	0.597
4700	61.066	365.415	313.468	244.155	−904.766	−34.070	0.379
4800	61.138	366.702	314.563	250.265	−906.973	−15.521	0.169
4900	61.203	367.963	315.640	256.382	−909.190	3.073	−0.033
5000	61.262	369.200	316.699	262.505	−911.420	21.714	−0.227
5100	61.315	370.414	317.740	268.634	−913.662	40.399	−0.414
5200	61.362	371.605	318.765	274.768	−915.917	59.127	−0.594
5300	61.404	372.774	319.773	280.907	−918.186	77.900	−0.768
5400	61.441	373.922	320.765	287.049	−920.470	96.716	−0.936
5500	61.472	375.050	321.742	293.195	−922.770	115.573	−1.098
5600	61.499	376.158	322.704	299.343	−925.087	134.474	−1.254
5700	61.522	377.247	323.651	305.494	−927.422	153.415	−1.406
5800	61.541	378.317	324.584	311.648	−929.775	172.398	−1.553
5900	61.555	379.369	325.504	317.802	−932.147	191.420	−1.695
6000	61.566	380.404	326.410	323.959	−934.539	210.484	−1.832

PREVIOUS: December 1975 (1 atm) CURRENT: December 1975 (1 bar)

Boric Acid (HBO_2) **CRYSTAL(I)** **$M_r = 43.81674$** **Boric Acid (HBO_2)** **$B_1H_1O_2(cr)$**

$\Delta_f H°(0\ K)$ = Unknown

$S°(298.15\ K) = [48.95 \pm 4.2]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_f H°(298.15\ K) = -802.8 \pm 0.84\ kJ{\cdot}mol^{-1}$

$T_{fus} = 509 \pm 1\ K$ $\Delta_{fus}H°$ = Unknown

Enthalpy of Formation

The enthalpy change ($\Delta_r H°$) of the reaction $HBO_2(cr, I) + H_2O(l) = H_3BO_3(cr)$ has been determined Kilday.[1] From the value, $\Delta_r H°(298.15\ K) = -1.28\ kcal{\cdot}mol^{-1}$, the enthalpy of formation $\Delta_f H°(298.15\ K)$ for HBO_2 (cr, I) is derived to be $-191.87 \pm 0.20\ kcal{\cdot}mol^{-1}$ which is adopted. The enthalpies of solution of HBO_2 (cr, I) in $H_2O(l)$ were measured by Sokolova, *et al.*[2] Based on the reported value, $\Delta_r H°(298.15\ K) = 1.76 \pm 0.01\ kcal\ mol^{-1}$ for the reaction $HBO_2(cr, I) + 501\ H_2O(l) = H_3BO_3{\cdot}500\ H_2O(Sol)$, the enthalpy of formation for HBO_2(cr, I) was derived as $-189.46 \pm 0.20\ kcal{\cdot}mol^{-1}$, using $\Delta_f H°(H_2O, l, 298.15\ K) = -68.317$ and $\Delta_f H°(H_3BO_3{\cdot}500\ H_2O$, Sol, 298.15 K), $= -256.02 \pm 0.20\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

The values of heat capacity for HBO_2(cr, I) were estimated by comparison with those of its constituent oxides. $S°(298.15\ K)$ was calculated as the sum of the entropy contributions from H^+ and BO_2^- in HBO_2(c) suggested by Kelley and Kubaschewski and Evans.

Fusion Data

Kracek, Morey and Merwin reported the existence of three crystal forms of HBO_2(c), namely HBO_2(cr, I), $T_{fus} = 509 \pm 1K$; HBO_2(cr, II), $T_{fus} = 474.1 \pm 0.5\ K$; and HBO_2(cr, III), $T_{fus} = 449.2 \pm 0.2\ K$. However, there was no solid phase equilibrium found among these crystals. Sokolova, Skuratov, Shemonaeva and Yuldasheva measured the enthalpies of solution in water of HBO_2(cr, I) and HBO_2(cr, II) and derived the enthalpy of transition as $\Delta_{trs}H°(II \rightarrow I, 298.15\ K) = 1.29\ kcal{\cdot}mol^{-1}$.

Sublimation Data

The value of $\Delta_{sub}H°(298.15\ K)$ is calculated as the difference between the $\Delta_f H°(298.15\ K)$ values for HBO_2(g) and HBO_2(c).

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Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	54.392	48.953	48.953	.000	−802.784	−734.994	128.768
300	54.810	49.291	48.954	.101	−802.785	−734.574	127.901
400	61.505	66.015	51.189	5.931	−802.742	−711.839	92.957
500	66.526	80.279	55.615	12.332	−802.592	−689.128	71.993
600	71.546	92.835	60.791	19.227	−802.303	−666.460	58.020
700	78.921	104.435	66.205	26.761	−801.647	−643.864	48.046
800	84.935	115.381	71.675	34.965	−800.539	−621.395	40.573
900	89.642	125.671	77.109	43.706	−799.072	−599.086	34.770
1000	92.885	135.297	82.452	52.845	−797.360	−576.956	30.137
1100	94.056	144.207	87.667	62.194	−795.569	−555.002	26.355
1200	94.977	152.432	92.725	71.648	−793.792	−533.211	23.210
1300	95.646	160.062	97.615	81.181	−792.044	−511.567	20.555
1400	96.065	167.167	102.332	90.769	−790.341	−490.056	18.284
1500	96.232	173.802	106.878	100.386	−788.704	−468.665	16.320

PREVIOUS: September 1962 CURRENT: December 1964

Boric Acid (HBO_2) **$B_1H_1O_2(cr)$**

Boric Acid (HBO_2) IDEAL GAS $M_r = 43.81674$ Boric Acid (HBO_2) $B_1H_1O_2(g)$

$S°(298.15\ K) = [239.73]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -557.2 \pm 4.2\ kJ{\cdot}mol^{-1}$

$\Delta_fH°(298.15\ K) = -560.7 \pm 4.2\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}	υ, cm^{-1}
3680(1)	[1250](1)
2030(1)	[600](1)
1420(1)	[700](1)

Ground State Quantum Weight: 1 $\sigma = 1$

Point Group: [C_s]

Bond Distances: H–O = [1.0] Å; O–B = [1.34] Å; B–O = [1.20] Å

Bond Angles: H–O–B = [120]°; O–B–O = [180]°

Product of the Moments of Inertia: $I_AI_BI_C = [9.70076 \times 10^{-117}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The equilibrium pressures of the reaction $1/2\ B_2O_3(l) + 1/2\ H_2O(g) = HBO_2(g)$ have been measured by several investigators. Using the equilibrium data reported, the enthalpies of reaction, $\Delta_rH°(298.15\ K)$, were evaluated by both the 2nd and 3rd law methods. The corresponding enthalpies of formation for $HBO_2(g)$ were derived based on the $\Delta_rH°(298.15\ K)$ values obtained by the 3rd law method. The results are presented as follows:

Source	T/K	$\Delta_rH°(298.15\ K)$, $kcal{\cdot}mol^{-1}$ 2nd law	3rd law	$\Delta_fH°(298.15\ K)$ $kcal{\cdot}mol^{-1}$
[1]	1061 – 1451	45.4 ± 0.6	45.16	−133.38 ± 0.50
	1323 – 1451	0.25 ± 6.0	−5.15	−133.62 ± 0.50
[2]	1250 – 1450	39.7 ± 2.5	—	−138.87 ± 2.50*
[3]	1273	—	44.12	−134.42 ± 1.0
[4]	1070 – 1323	31.0 ± 10.0	44.07	−134.47 ± 3.20
	1143	—	40.9	−137.64 ± 0.70*
	1071 – 1325	44.2 ± 1.8	39.3	−139.3 ± 1.0*
	1148	—	43.2	−135.3 ± 0.4

*The value not used for the calculation of the weighted average of $\Delta_fH°(298.15\ K)$ for $HBO_2(g)$

Heat Capacity and Entropy

All molecular and spectroscopic constants were taken from White and Mann *et al.*[2] The principal moments of inertia are: $I_A = 0.1155 \times 10^{-39}$, $I_B = 9.1066 \times 10^{-39}$ and $I_C = 9.2221 \times 10^{-39}\ g{\cdot}cm^2$.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−10.687	−557.212	−557.212	INFINITE
100	33.404	200.044	273.638	−7.359	−558.313	−555.919	290.382
200	36.887	224.017	243.422	−3.881	−559.425	−553.107	144.457
250	39.583	232.535	240.414	−1.970	−560.041	−551.456	115.221
298.15	42.232	239.734	239.734	0.	−560.656	−549.748	96.313
300	42.332	239.995	239.735	0.078	−560.680	−549.680	95.708
350	45.007	246.723	240.260	2.262	−561.324	−547.796	81.754
400	47.553	252.901	241.459	4.577	−561.968	−545.819	71.277
450	49.941	258.641	243.053	7.015	−562.605	−543.762	63.118
500	52.157	264.019	244.883	9.568	−563.228	−541.635	56.584
600	56.073	273.885	248.910	14.985	−564.416	−537.203	46.768
700	59.364	282.783	253.124	20.762	−565.518	−532.579	39.742
800	62.136	290.896	257.345	26.841	−566.535	−527.803	34.462
900	64.489	298.354	261.493	33.175	−567.476	−522.904	30.349
1000	66.505	305.256	265.529	39.727	−568.349	−517.905	27.053
1100	68.244	311.678	269.436	46.467	−569.168	−512.820	24.352
1200	69.752	317.682	273.209	53.368	−569.944	−507.663	22.098
1300	71.066	323.318	276.849	60.411	−570.686	−502.443	20.188
1400	72.215	328.628	280.359	67.576	−571.406	−497.166	18.549
1500	73.223	333.645	283.746	74.849	−572.113	−491.839	17.127
1600	74.111	338.400	287.015	82.216	−572.814	−486.464	15.881
1700	74.894	342.917	290.171	89.668	−573.518	−481.046	14.781
1800	75.588	347.218	293.222	97.192	−574.231	−475.586	13.801
1900	76.203	351.321	296.173	104.782	−574.958	−470.086	12.924
2000	76.752	355.244	299.029	112.431	−575.705	−464.547	12.133
2100	77.242	359.001	301.796	120.131	−576.475	−458.970	11.416
2200	77.681	362.605	304.479	127.877	−577.273	−453.356	10.764
2300	78.075	366.067	307.082	135.666	−578.102	−447.705	10.168
2400	78.430	369.397	309.609	143.491	−629.224	−440.949	9.597
2500	78.751	372.605	312.065	151.350	−630.199	−433.084	9.049
2600	79.041	375.700	314.454	159.240	−631.179	−425.180	8.542
2700	79.305	378.688	316.778	167.158	−632.166	−417.238	8.072
2800	79.545	381.576	319.041	175.100	−633.161	−409.259	7.635
2900	79.764	384.372	321.245	183.066	−634.165	−401.246	7.227
3000	79.964	387.079	323.395	191.053	−635.179	−393.196	6.846
3100	80.148	389.704	325.492	199.058	−636.204	−385.113	6.489
3200	80.316	392.252	327.539	207.082	−637.240	−376.997	6.154
3300	80.472	394.725	329.537	215.121	−638.288	−368.849	5.838
3400	80.615	397.130	331.490	223.176	−639.349	−360.668	5.541
3500	80.747	399.469	333.399	231.244	−640.422	−352.456	5.260
3600	80.869	401.745	335.266	239.325	−641.508	−344.213	4.994
3700	80.982	403.962	337.093	247.417	−642.607	−335.940	4.743
3800	81.088	406.123	338.881	255.521	−643.719	−327.636	4.504
3900	81.185	408.231	340.632	263.635	−644.844	−319.303	4.277
4000	81.277	410.288	342.348	271.758	−645.982	−310.942	4.060
4100	81.362	412.296	344.030	279.890	−647.134	−302.551	3.855
4200	81.441	414.257	345.679	288.030	−1128.149	−287.109	3.571
4300	81.516	416.174	347.296	296.178	−1128.242	−267.082	3.244
4400	81.585	418.049	348.883	304.333	−1128.350	−247.055	2.933
4500	81.651	419.883	350.440	312.495	−1128.474	−227.025	2.635
4600	81.712	421.679	351.969	320.663	−1128.615	−206.991	2.350
4700	81.770	423.437	353.471	328.837	−1128.774	−186.954	2.078
4800	81.824	425.159	354.947	337.017	−1128.950	−166.913	1.816
4900	81.876	426.846	356.397	345.202	−1129.146	−146.868	1.566
5000	81.924	428.501	357.823	353.392	−1129.360	−126.819	1.325
5100	81.970	430.124	359.225	361.586	−1129.595	−106.766	1.094
5200	82.013	431.716	360.603	369.786	−1129.850	−86.709	0.871
5300	82.054	433.279	361.960	377.989	−1130.127	−66.645	0.657
5400	82.092	434.813	363.295	386.196	−1130.427	−46.577	0.451
5500	82.129	436.319	364.609	394.407	−1130.750	−26.504	0.252
5600	82.164	437.799	365.903	402.622	−1131.098	−6.422	0.060
5700	82.197	439.254	367.177	410.840	−1131.472	13.664	−0.125
5800	82.229	440.684	368.432	419.061	−1131.872	33.758	−0.304
5900	82.258	442.090	369.668	427.286	−1132.299	53.857	−0.477
6000	82.287	443.473	370.887	435.513	−1132.756	73.966	−0.644

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Boron Hydride Sulfide (HBS) IDEAL GAS $M_r = 43.87794$ Boron Hydride Sulfide (HBS) $B_1H_1S_1(g)$

$S°(298.15\ K) = [214.96 \pm 0.4]\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = [50.8 \pm 10.0]\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [50.2 \pm 10.0]\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights

ϵ_i, cm^{-1}	g_i	ϵ_i, cm^{-1}	g_i
0	[1]	[35000]	[1]
[25000]	[3]	[37000]	[2]
[30000]	[6]	[40000]	[6]
[31000]	[3]		

Vibrational Frequencies and Degeneracies
υ, cm^{-1}

2742(1)
[715](2)
[1156](1)

Point Group: $C_{\infty v}$ $\sigma = 1$
Bond Distances: H–B = 1.1692 Å; B–S = 1.5994 Å
Bond Angle: H–B–S = 180°
Rotational constant: $B_0 = 0.643679\ cm^{-1}$

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
0	0.	0.	INFINITE	−9.287	50.781	50.781	INFINITE
100	29.161	180.556	244.344	−6.379	51.475	39.739	−20.758
200	31.839	201.339	218.167	−3.366	51.167	28.051	−7.326
250	34.328	208.706	215.556	−1.713	50.731	22.320	−4.664
298.15	36.789	214.964	214.964	0.	50.208	16.894	−2.960
300	36.881	215.192	214.965	0.068	50.186	16.688	−2.906
350	39.237	221.057	215.422	1.972	49.573	11.152	−1.664
400	41.313	226.435	216.468	3.987	46.693	5.797	−0.757
450	43.113	231.408	217.855	6.099	45.321	0.758	−0.088
500	44.673	236.033	219.444	8.294	43.880	−4.114	0.430
600	47.240	244.414	222.922	12.895	41.450	−13.478	1.173
700	49.284	251.855	226.534	17.725	39.309	−22.460	1.676
800	50.966	258.549	230.124	22.740	37.354	−31.149	2.034
900	52.379	264.636	233.626	27.909	−17.603	−38.520	2.236
1000	53.577	270.219	237.010	33.209	−18.124	−40.816	2.132
1100	54.598	275.374	240.266	38.619	−18.634	−43.061	2.045
1200	55.470	280.163	243.394	44.123	−19.145	−45.259	1.970
1300	56.219	284.633	246.396	49.709	−19.664	−47.414	1.905
1400	56.863	288.824	249.278	55.364	−20.199	−49.529	1.848
1500	57.419	292.766	252.047	61.078	−20.756	−51.605	1.797
1600	57.901	296.488	254.710	66.845	−21.339	−53.642	1.751
1700	58.320	300.011	257.272	72.657	−21.953	−55.643	1.710
1800	58.686	303.355	259.740	78.507	−22.601	−57.606	1.672
1900	59.008	306.537	262.120	84.392	−23.283	−59.532	1.637
2000	59.291	309.571	264.417	90.308	−24.002	−61.421	1.604
2100	59.541	312.470	266.637	96.249	−24.758	−63.274	1.574
2200	59.763	315.245	268.784	102.215	−25.551	−65.090	1.545
2300	59.961	317.906	270.862	108.201	−26.383	−66.868	1.519
2400	60.139	320.462	272.876	114.206	−77.513	−67.541	1.470
2500	60.299	322.920	274.829	120.228	−78.499	−67.106	1.402
2600	60.444	325.288	276.724	126.266	−79.492	−66.630	1.339
2700	60.576	327.572	278.565	132.317	−80.490	−66.117	1.279
2800	60.697	329.777	280.355	138.380	−81.494	−65.566	1.223
2900	60.810	331.909	282.096	144.456	−82.504	−64.979	1.170
3000	60.915	333.972	283.791	150.542	−83.520	−64.358	1.121
3100	61.016	335.971	285.443	156.639	−84.541	−63.702	1.073
3200	61.112	337.910	287.052	162.745	−85.569	−63.014	1.029
3300	61.207	339.792	288.622	168.861	−86.601	−62.293	0.986
3400	61.301	341.620	290.154	174.987	−87.639	−61.541	0.945
3500	61.396	343.399	291.650	181.121	−88.682	−60.758	0.907
3600	61.493	345.130	293.111	187.266	−89.730	−59.945	0.870
3700	61.594	346.816	294.540	193.420	−90.781	−59.103	0.834
3800	61.701	348.460	295.938	199.585	−91.836	−58.233	0.800
3900	61.814	350.064	297.305	205.761	−92.894	−57.335	0.768
4000	61.935	351.631	298.644	211.948	−93.955	−56.410	0.737
4100	62.066	353.162	299.955	218.148	−95.017	−55.458	0.707
4200	62.206	354.659	301.239	224.361	−575.929	−47.456	0.590
4300	62.359	356.124	302.499	230.590	−575.903	−34.874	0.424
4400	62.524	357.560	303.734	236.834	−575.878	−22.292	0.265
4500	62.703	358.967	304.946	243.095	−575.852	−9.711	0.113
4600	62.897	360.347	306.135	249.375	−575.824	2.870	−0.033
4700	63.106	361.702	307.303	255.675	−575.793	15.450	−0.172
4800	63.331	363.033	308.450	261.996	−575.757	28.029	−0.305
4900	63.574	364.341	309.578	268.342	−575.716	40.607	−0.433
5000	63.833	365.628	310.686	274.712	−575.667	53.185	−0.556
5100	64.111	366.895	311.776	281.109	−575.609	65.762	−0.674
5200	64.407	368.143	312.848	287.535	−575.541	78.337	−0.787
5300	64.721	369.372	313.903	293.991	−575.461	90.911	−0.896
5400	65.054	370.585	314.941	300.479	−575.366	103.483	−1.001
5500	65.405	371.782	315.964	307.002	−575.256	116.053	−1.102
5600	65.774	372.964	316.971	313.561	−575.129	128.621	−1.200
5700	66.162	374.132	317.964	320.158	−574.982	141.187	−1.294
5800	66.567	375.286	318.942	326.794	−574.814	153.750	−1.385
5900	66.989	376 427	319.907	333.471	−574.623	166.310	−1.472
6000	67.428	377.557	320.858	340.192	−574.408	178.866	−1.557

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

PREVIOUS: December 1975 (1 atm) CURRENT· December 1975 (1 bar)

Enthalpy of Formation

The transient thioborine molecule, HBS, has been identified by Kirk and Timms[1] in the mass spectra of the products fromed by the high temperature (1150–1300°C) reaction of hydrogen sulfide on crystalline boron. The best yields of HBS were found at low pressures (<1 torr) but even under thses conditions the half-life is relatively short (<3 min).[1, 2] No experimental measurement of its enthalpy of formation has been reported.

We estimate $\Delta_f H°$ from a consideration of bond–energy schemes. A comparison of the values for the H–B stretching force constants in HBS ($K = 4.021 \times 10^5$ dynes/cm) and HBO ($K = 4.080 \times 10^5$ dynes/cm)[3] suggests that the H–B bonds in these two molecules are quite similar. Assuming $\Delta_a H°$(H–BO, 298.15 K) = 99.5 kcal·mol^{-1},[3] we calculate $\Delta_f H°$(298.15 K) = 10.7 kcal·mol^{-1}with $\Delta_f H°$(H, g, 298.15 K) = 52.103 kcal·mol^{-1} and $\Delta_f H°$(BS, g 298.15 K) = 58.1 ± 4.0 kcal·mol^{-1}.[3]

A comparison of force constants also suggests that the H–B bonds in BH_3[4] and the B=S bond in BS[3] are similar to those in HBS. Using $\Delta_a H°$(H–B, 298.15 K) = $\Delta_a H°$(BH_3, g, 298.15 K)/3 = 87.9 kcal·mol^{-1} and $\Delta_a H°$(B=S, 298.15 K) = $\Delta_a H°$(BS, 298.15 K) = 141.0 kcal·mol^{-1}, we calculate $\Delta_a H°$(298.15 K) = 228.9 kcal·mol^{-1} which leads to $\Delta_f H°$(298.15 K) = 22.3 kcal·mol^{-1}. All bond dissociation energies are derived from JANAF data.[3]

A value for $\Delta_a H°$(298.15 K) can also be obtained from the results of MO calculations on HBS. Thomson[5] has shown that dissociation energies obtained from MO calculations when combined with estimates of the molecular extra correlation energy (MECE) give reliable atomization energies. The change in the relativistic energy between the isolated atoms and molecule is assumed small. It is reasonable to assume that the contribution to the atomization energy from correlation effects would be similar for the isoelectronic molecules HBS and HBO. We estimate the MECE for HBO as 56.5 kcal·mol^{-1} from the difference in the experimental $\Delta_a H°$[3] and the reported Hartree–Fock dissociation energy.[6] This value of MECE when added to the computed dissociation energy[7] of 191.7 kcal·mol^{-1} gives $\Delta_a H°$(298.15 K) = 248.2 kcal·mol^{-1} which corresponds to $\Delta_f H°$(HBS, g, 298.15 K) = 3.0 kcal·mol^{-1} We believe these three estimates of $\Delta_f H°$(10.7, 22.3, 3.0 kcal·mol^{-1}) to be equally probable; therefore, we adopt the mean value of 12 0 kcal·mol^{-1}. An uncertainty of ±10.0 kcal·mol^{-1} is assigned which covers the range of possible values.

Heat Capacity and Entropy

The microwave measurements on HBS by Pearson and McCormick[8] have shown that the molecule is linear in its ground state. They observed the millimeter–wave spectra for eight isotopic species and evaluated structural parameters by the substitution method. We adopt their mean values for the H–B and B=S bond lengths.

Sams and Maki[2] have observed the υ_1 vibrational fundamental (2742 cm^{-1}) in the high–resolution infrared spectra of HBS(g). Frequencies (υ_1) were recorded for four isotopic species. The value of υ_1(2742 cm^{-1}) is corrected for the natural isotopic abundances of boron: the correction for the sulfur isotopes is negligible. Values of υ_2 and υ_3 are calculated from force constants by a valence force method.[9] The B=S stretching force constant ($K = 6.9 \times 10^5$ dynes/cm) is estimated from the value for BS ($K = 6.7 \times 10^5$ dynes/cm) by comparison with the B=O stretching force constants for BO and HBO.[3] The bending force constant ($K_D = 3.2 \times 10^{12}$ dynes/cm) is taken equal to the value for HBO.[3] Sams and Maki[2] also performed a detailed force field calculation on HBS which gave $\upsilon_2 = 635$ cm^{-1} for $H^{11}B^{32}S$. Results of a similar

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Boron Hydride Sulfide (HBS) $B_1H_1S_1(g)$

Boron Hydride Sulfide, Ion (HBS⁺) IDEAL GAS $M_r = 43.87739$ Boron Hydride Sulfide, Ion (HBS⁺) $B_1H_1S_1^+(g)$

$S°(298.15\ K) = [225.4 \pm 0.4]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = [1123.2 \pm 11]\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = [1129.5 \pm 11]\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$X^2\Pi_{1/2}$	0	2
$X^2\Pi_{3/2}$	[300]	2
$A^2\Sigma^+$	19599	2
$B^2\Sigma^+$	38069	2

Vibrational Frequencies and Degeneracies υ, cm^{-1}
[2550](1)
[764](2)
973 (1)

Point Group: $C_{\infty v}$ $\sigma = 1$
Bond Distances: H–B = [1.192] Å; B–S = [1.680] Å
Bond Angle: H–B–S = 180°
Rotational Constant. B_o = [0.586979] cm^{-1}

Enthalpy of Formation

Kroto *et al.*[1] and Fehler and Turner[2] have independently measured the 584 Å photoelectron spectra of HBS(g). The reported value of 11.11 ± 0.03 eV[1] and 11.12 eV[2] for the first adiabatic ionization potential are in excellent agreement. We adopt an average (11.115 ± 0.03 eV) of these two IP values, and we assume $\Delta_rH° = 256.32 \pm 0.7$ kcal·mol^{-1} refers to the ionization process $HBS(g) + e^- + HBS^+(g) + 2\,e^-$ at 0 K. The latter value yields $\Delta_fH°(HBS^+, g, 0\ K) = 268.4 \pm 11.0$ kcal·mol^{-1} when combined with $\Delta_fH°(HBS, g, 0\ K) = 12.1 \pm 10.0$ kcal·mol^{-1}.[3] The adopted $\Delta_fH°$ value is placed in brackets to emphasize the uncertainty in the estimated $\Delta_fH°$ value[3] for HBS. $\Delta_fH°(298.15\ K)$ corresponds to 270.0 ± 11.0 kcal·mol^{-1}.

Heat Capacity and Entropy

Extensive ab initio MO calculations[4] recently reported for HBS show that the highest occupied orbital is of Π–symmetry and is localized mainly on the sulfur atom. The shape of the first photoelectron band in the HBS spectra[1 2] suggests that this orbital is bonding. The bonding nature of this Π orbital is also predicted from the Walsh diagram[5] for HAB molecules. As a consequence, we would expect the ion to be less strongly bound than the parent molecule. In the related species HCN[6] which has the same orbital ordering as HBS,[4] ionization[7] occurs with a 2.2% increase in the H–C bond length and a 4.7% increase in the C≡N bond length. We assume a similar increase in the bond lengths of HBS[3] upon ionization. If the ion was nonlinear, one would expect to find a vibrational spacing in the photoelectron spectra of HBS which could be associated with the bending frequency of the ion. No frequency as low as 764 cm^{-1} has been observed,[1 2] thus, it is likely that HBS⁺ is linear in its ground state. This prediction is supported by the Walsh diagram.[5] We assume that the ion is linear.

The progression in the first photoelectron band of the HBS spectra has been reported as 955 ± 40 cm^{-1} [1] and 990 cm^{-1}.[2] By comparison with changes observed in vibrational frequencies on ionization of HCN and HCP,[1 8] the vibrational mode excited is most certainly the B=S stretching frequency, υ_3. We adopt the average (973 cm^{-1}) of these two values. The values of υ_1 and are calculated from estimated force constants by a valence force method.[9] The two force constants are estimated form those for HCN⁺,[8] NCH and NBS.[3] We estimate the uncertainties in our frequencies are no greater than ±50 cm^{-1} which corresponds to an error in the value of $S°(298.15\ K)$ of only ±0.12 kcal·mol^{-1}.

The electronic states and upper levels are taken from the photoelectron spectrometric study of Kroto *et al.*[1] Relative term values for the $A^2\Sigma^+$ and $B^2\Sigma^+$ states are calculated as differences in the reported adiabatic ionization potentials.[1] Fehler and Turner[2] have estimated the ground state splitting to be ~300 cm^{-1} from the observed peak widths in the first band of the HBS photoelectron spectra. We adopt this result since it compares favorably with the splitting (~278 cm^{-1}) observed for the $^2\Pi$ state of the isoelectronic molecules CS⁺.[10] Relative term values for the two $^2\Sigma$ states calculated from the adiabatic ionization potentials of Fehler and Turner[2] agree within about 160 cm^{-1} with the values adopted here. Fehler and Turner[2] have also reported a photoelectron band at 17 9 eV which was not observed by Kroto *et al.*[1] This band could not be definitely assigned to HBS⁺. If this state does exist, it lies above 50000 cm^{-1} and has a negligible effect on the thermodynamic functions of the ion. We prefer not to include it. Kroto *et al.*[1] have interpreted their photoelectron results in terms of a linear configuration for the three observed states of HBS⁺. Thus, we feel our functions are not significantly influenced by the use of the ground state vibrational frequencies and rotational constant for the excited states.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−9.934	1123.199		
100	31.149	187.666	257.455	−6.979			
200	35.146	210.523	228.818	−3.659			
250	37.309	218.594	225.988	−1.848			
298.15	39.455	225.350	225.350	0.	1129.471	1086.806	−190.404
300	39.535	225.594	225.351	0.073	1129.493	1086.541	−189.184
350	41.615	231.848	225.840	2.103	1130.044	1079.338	−161.082
400	43.459	237.528	226.951	4.231	1128.316	1072.148	−140.008
450	45.064	242.741	228.420	6.445	1128.086	1065.132	−123.637
500	46.464	247.563	230.096	8.734	1127.777	1058.156	−110.545
600	48.787	256.248	233.747	13.501	1127.593	1044.255	−90.910
700	50.657	263.914	237.520	18.476	1127.676	1030.362	−76.887
800	52.207	270.783	241.256	23.621	1127.929	1016.444	−66.367
900	53.508	277.009	244.888	28.909	1075.170	1003.568	−58.246
1000	54.607	282.705	248.389	34.316	1076.835	995.523	−52.001
1100	55.538	287.955	251.750	39.825	1078.502	987.311	−46.883
1200	56.329	292.822	254.973	45.419	1080.160	978.948	−42.612
1300	57.004	297.358	258.061	51.087	1081.801	970.447	−38.993
1400	57.581	301.604	261.021	56.817	1083.420	961.820	−35.886
1500	58.076	305.594	263.861	62.600	1085.011	953.079	−33.189
1600	58.503	309.356	266.588	68.430	1086.568	944.232	−30.826
1700	58.873	312.914	269.209	74.299	1088.091	935.289	−28.738
1800	59.195	316.289	271.732	80.203	1089.575	926.258	−26.879
1900	59.477	319 497	274.162	86.137	1091.020	917.145	−25.214
2000	59.725	322.554	276.506	92.097	1092.425	907.957	−23.713
2100	59.943	325.474	278.769	98.081	1093.790	898.700	−22.354
2200	60.137	328.267	280.955	104.085	1095.114	889.379	−21.117
2300	60.309	330.944	283.071	110.107	1096.396	879.999	−19.985
2400	60.464	333.514	285.120	116.146	1047.379	871.632	−18.971
2500	60.603	335.985	287.105	122.200	1048.502	864.286	−18.058
2600	60.729	338.364	289.031	128.266	1049.618	856.895	−17.215
2700	60.844	340.659	290.901	134.345	1050.726	849.462	−16.434
2800	60.949	342.873	292.718	140.435	1051.827	841.988	−15.707
2900	61.046	345.014	294.485	146.535	1052.920	834.474	−15.031
3000	61.136	347.085	296.204	152.644	1054.005	826.923	−14.398
3100	61.220	349.091	297.877	158.762	1055.083	819.336	−13.806
3200	61.299	351.036	299.508	164.887	1056.154	811.714	−13.250
3300	61.373	352.923	301.099	171.021	1057.218	804.059	−12.727
3400	61.444	354.756	302.650	177.162	1058.274	796.371	−12.235
3500	61.512	356.538	304.164	183.310	1059.323	788.653	−11.770
3600	61.577	358.272	305.643	189.464	1060.364	780.905	−11.331
3700	61.641	359.960	307.089	195.625	1061.398	773.128	−10.915
3800	61.702	361.605	308.502	201.792	1062.423	765.323	−10.520
3900	61.762	363.208	309.884	207.966	1063.442	757.491	−10.145
4000	61.821	364.773	311.237	214.145	1064.452	749.633	−9.789
4100	61.879	366.300	312.561	220.330	1065.453	741.750	−9.450
4200	61.937	367.792	313.858	226.521	586.597	740.867	−9.214
4300	61.993	369.250	315.130	232.717	588.670	744.516	−9.044
4400	62.049	370.676	316.376	238.919	590.732	748.116	−8.881
4500	62.105	372.071	317.598	245.127	592.783	751.670	−8.725
4600	62.160	373.437	318.797	251.340	594.823	755.178	−8.575
4700	62.216	374.774	319.974	257.559	596.851	758.643	−8.431
4800	62.270	376.084	321.129	263.783	598.868	762.064	−8.293
4900	62.325	377.369	322.264	270.013	600.873	765.443	−8.160
5000	62.380	378.629	323.379	276.248	602.865	768.781	−8.031
5100	62.434	379.864	324.474	282.489	604.845	772.080	−7.908
5200	62.488	381.077	325.551	288.735	606.813	775.340	−7.788
5300	62.542	382.268	326.610	294.987	608.767	778.562	−7.673
5400	62.596	383.438	327.652	301.244	610.708	781.747	−7.562
5500	62.649	384.587	328.677	307.506	612.636	784.897	−7.454
5600	62.703	385.716	329.685	313.773	614.551	788.012	−7.350
5700	62.756	386.826	330.678	320.046	616.453	791.092	−7.250
5800	62.808	387 918	331.655	326.325	618.341	794.140	−7.152
5900	62.861	388.992	332.618	332.608	620.216	797.155	−7.057
6000	62.913	390.049	333.566	338.897	622.078	800.138	−6.966

PREVIOUS: December 1975 (1 atm) CURRENT· December 1975 (1 bar)

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Borane (BH$_2$) IDEAL GAS M_r = 12.82588 Borane (BH$_2$) B$_1$H$_2$(g)

$S°$(298.15 K) = [180.19] J·K^{-1}·mol^{-1}

$\Delta_f H°$(0 K) = 202 ± 63 kJ·mol^{-1}
$\Delta_f H°$(298.15 K) = 201 ± 63 kJ·mol^{-1}

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
[2430]	[840](2)	[2650](1)

Ground State Quantum Weight: [2] $\sigma = 2$
Point Group: [$D_{\infty h}$]
Bond Distance: B–H = [1.20] Å
Bond Angle: H–B–H = [180]°
Rotational Constant. B_0 = [5.807235] cm^{-1}

Enthalpy of Formation

$\Delta_f H°$(298.15 K) was calculated from appearance potentials reported by Fehlner and Koski[1] and the JANAF Thermochemical Table.[2] For example:

	$\Delta_r H°$(0 K)
$B_2H_6(g) \rightarrow BH_{2+}(ion) + BH_2(g) + H_2(g)$	13.4 eV
$BH_2(g) \rightarrow BH_2+(ion)$	9.8 eV
$B_2H_6(g) \rightarrow 2\ BH_2(g) + H_2(g)$	3.6 eV

The $\Delta_f H°$ data is summarized below.

Source	Method	$\Delta_f H°$(298.15 K), kcal·mol^{-1}
[2]	Appearance Potentials	48
[3]	Estimate	66
[4]	Estimate	93

Heat Capacity and Entropy

The bond distance B–H = 1.20 Å was estimated from a consideration of BH(g), BH$_3$(g) and other molecules. The bond angle H–B–H = 180° and the electronic configuration of the ground state [$^2A_2$] were estimated by Jordan and Longuet Higgins.[4] The frequencies were estimated assuming valence forces, Herzberg,[5] and using force constants, $k_1 = 3.5 \times 10^5$ dynes cm^{-1} and $k\delta\, l^1 = 0.35 \times 10^5$ dynes cm^{-1}, estimated from BH$_3$, Shepp and Bauer.[6]

References

[1] T. P. Fehlner and W. S. Koski, J. Am. Chem. Soc. 86, 2733 (1964).
[2] JANAF Thermochemical Tables: B$_2$H$_6$(g), 12-31-64.
[3] C. J. O'Brien and J. R. Perrin, Marquardt Corp., Van Nuys, California and J. Perine, Olin Mathieson Chemical Corp., New York, Estimation of the Heats of Formation of Gaseous Combustion Product Molecules, (October 1959).
[4] P. C. H. Jordan and H. C. Longuet Higgins, Mol. Phys. 5, 121 (1962).
[5] G. Herzberg, "Molecular Spectra and Molecular Structure II Infrared and Raman Spectra of Polyatomic Molecules," D. Van Nostrand Co., Inc., New York, pp 172 (1945).
[6] A. Shepp and S. H. Bauer, J. Am. Chem. Soc. 76, 265 (1954).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−9.008	201.505	201.505	INFINITE
100	29.115	146.922	208.138	−6.122	201.368	196.780	−102.787
200	30.550	167.371	183.190	−3.164	201.300	192.192	−50.195
250	32.243	174.363	180.745	−1.595	201.101	189.935	−39.685
298.15	34.026	180.195	180.195	0.	200.832	187.809	−32.903
300	34.094	180.405	180.195	0.063	200.821	187.728	−32.686
350	35.849	185.795	180.617	1.812	200.494	185.571	−27.695
400	37.432	190.687	181.574	3.645	200.134	183.463	−23.958
450	38.855	195.179	182.840	5.553	199.754	181.402	−21.057
500	40.154	199.341	184.284	7.528	199.364	179.384	−18.740
600	42.509	206.874	187.435	11.664	198.589	175.461	−15.275
700	44.645	213.590	190.700	16.023	197.855	171.665	−12.810
800	46.593	219.681	193.948	20.587	197.183	167.970	−10.967
900	48.350	225.272	197.122	25.335	196.576	164.356	−9.539
1000	49.913	230.449	200.199	30.250	196.025	160.806	−8.400
1100	51.287	235.272	203.170	35.312	195.517	157.309	−7.470
1200	52.487	239.787	206.036	40.502	195.040	153.857	−6.697
1300	53.531	244.030	208.797	45.804	194.580	150.444	−6.045
1400	54.439	248.032	211.458	51.203	194.126	147.066	−5.487
1500	55.228	251.815	214.023	56.688	193.668	143.720	−5.005
1600	55.916	255.402	216.498	62.246	193.198	140.406	−4.584
1700	56.517	258.810	218.888	67.868	192.711	137.121	−4.213
1800	57.043	262.056	221.197	73.546	192.201	133.865	−3.885
1900	57.505	265.153	223.429	79.274	191.664	130.639	−3.592
2000	57.913	268.113	225.590	85.046	191.098	127.442	−3.328
2100	58.274	270.947	227.683	90.855	190.500	124.274	−3.091
2200	58.595	273.666	229.712	96.699	189.868	121.135	−2.876
2300	58.880	276.277	231.680	102.573	189.200	118.025	−2.680
2400	59.136	278.788	233.591	108.474	138.236	116.014	−2.525
2500	59.366	281.207	235.447	114.399	137.417	115.105	−2.405
2600	59.572	283.539	237.252	120.347	136.591	114.229	−2.295
2700	59.759	285.791	239.009	126.313	135.758	113.385	−2.194
2800	59.927	287.968	240.718	132.298	134.918	112.571	−2.100
2900	60.081	290.073	242.384	138.298	134.070	111.788	−2.014
3000	60.220	292.112	244.008	144.313	133.213	111 035	−1.933
3100	60.348	294.089	245.592	150.342	132.347	110.309	−1.859
3200	60.464	296.007	247.137	156.383	131.470	109.613	−1.789
3300	60.571	297.869	248.647	162.434	130.584	108.943	−1.724
3400	60.669	299.679	250.121	168.496	129.687	108.301	−1.664
3500	60.760	301.439	251.562	174.568	128.778	107.685	−1.607
3600	60.843	303.152	252.972	180.648	127.859	107.095	−1.554
3700	60.921	304.820	254.351	186.737	126.927	106.531	−1.504
3800	60.992	306.446	255.700	192.832	125.984	105.993	−1.457
3900	61.059	308.031	257.022	198.935	125.028	105.479	−1.413
4000	61.120	309.577	258.316	205.044	124.060	104.990	−1.371
4100	61.178	311.087	259.585	211.159	123.079	104.526	−1.332
4200	61.232	312.562	260.829	217.279	−357.764	111.109	−1.382
4300	61.282	314.004	262.049	223.405	−357.684	122.272	−1.485
4400	61.329	315.413	263.246	229.536	−357.618	133.433	−1.584
4500	61.373	316.792	264.420	235.671	−357.568	144.593	−1.678
4600	61.414	318.141	265.574	241.810	−357.533	155.751	−1 769
4700	61.452	319.462	266.706	247.953	−357.513	166.909	−1.855
4800	61.489	320.756	267.819	254.100	−357.509	178.068	−1.938
4900	61.523	322.025	268.912	260.251	−357.521	189.225	−2.017
5000	61.555	323.268	269.987	266.405	−357.548	200.384	−2.093
5100	61.586	324.487	271.044	272.562	−357.591	211.542	−2.167
5200	61.614	325.683	272.083	278.722	−357.650	222.703	−2.237
5300	61.642	326.857	273.105	284.885	−357.724	233.864	−2.305
5400	61.667	328.010	274.112	291.050	−357.813	245.027	−2.370
5500	61.692	329.141	275.102	297.218	−357.917	256.191	−2.433
5600	61.715	330.253	276.077	303.389	−358.036	267.358	−2.494
5700	61.737	331.346	277.037	309.561	−358.169	278.527	−2.552
5800	61.758	332.420	277.982	315.736	−358.316	289.699	−2.609
5900	61.778	333.476	278.914	321.913	−358.476	300.872	−2.664
6000	61.796	334.514	279.832	328.091	−358.649	312.049	−2.717

PREVIOUS December 1964 (1 atm)   CURRENT· December 1964 (1 bar)

Dihydroxyborane (B(OH)$_2$) **IDEAL GAS** M_r = 44.82468 **Dihydroxyborane (B(OH)$_2$)** **B$_1$H$_2$O$_2$(g)**

$S°(298.15\ K) = [249.02]\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = [-470 \pm 15]\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [-477 \pm 15]\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}
[2500](1)	[750](1)	[1300](1)
[1150](1)	[460](1)	[1000](1)
[1100](1)	[3000](1)	[450](1)

Ground State Quantum Weight: [2] $\sigma = 2$
Point Group: [C_{2h}]
Bond Distances: B–O = [1.27] Å; O–H = [0.97] Å
Bond Angles: H–O–B = [105]°; O–B–O = [180]°
Product of the Moments of Inertia: $I_A I_B I_C = [24.2754 \times 10^{-117}]\ g^3 \cdot cm^6$

Enthalpy of Formation

The value of $\Delta_f H°(B(OH)_2, g, 298.15\ K)$ was calculated by using the bond energy, $D_0^°(B\text{–}OH) = 132.7\ kcal \cdot mol^{-1}$, and the enthalpies of formation for B(g) and OH(g) as 132.80 and 9.33 kcal·mol^{-1}, respectively.

Heat Capacity and Entropy

The vibrational frequencies were estimated by comparison with those for $BO_2(g)$, $B(OH)_3(g)$ and other related molecules. The bond distances and angles were estimated by comparison with those for $BO_2(g)$ and $H_2O_2(g)$ molecules. The molecular configuration is assumed to be trans which is considered as more stable than the cis–form. The principal moments of inertia are: $I_A = 0.2688 \times 10^{-39}$, $I_B = 9.3699 \times 10^{-39}$, and $I_C = 9.6387 \times 10^{-39}\ g \cdot cm^2$.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	.000	.000	INFINITE	−11.772	−470.383	−470.383	INFINITE
100	34.306	204.305	288.605	−8.430	−472.969	−465.966	243.395
200	42.381	230.309	253.468	−4.632	−475.109	−458.108	119.645
250	47.278	240.289	249.853	−2.391	−476.093	−453.742	94.804
298.15	52.015	249.023	249.023	.000	−476.976	−449.356	78.725
300	52.195	249.345	249.024	.096	−477.008	−449.185	78.210
350	56.883	257.747	249.677	2.825	−477.833	−444.481	66.335
400	61.190	265.629	251.183	5.778	−478.566	−439.665	57.414
450	65.065	273.064	253.205	8.936	−479.213	−434.763	50.466
500	68.519	280.102	255.546	12.278	−479.779	−429.793	44.900
600	74.344	293.129	260.743	19.432	−480.695	−419.705	36.539
700	79.038	304.954	266.227	27.109	−481.365	−409.484	30.556
800	82.894	315.768	271.753	35.212	−481.835	−399.181	26.064
900	86.106	325.723	277.204	43.666	−482.142	−388.829	22.567
1000	88.805	334.938	282.523	52.416	−482.321	−378.451	19.768
1100	91.088	343.513	287.682	61.414	−482.401	−368.059	17.478
1200	93.028	351.524	292.672	70.622	−482.408	−357.663	15.569
1300	94.683	359.037	297.491	80.010	−482.366	−347.269	13.953
1400	96.102	366.107	302.142	89.551	−482.292	−336.880	12.569
1500	97.324	372.780	306.631	99.224	−482.203	−326.497	11.370
1600	98.380	379.096	310.965	109.010	−482.111	−316.119	10.320
1700	99.298	385.088	315.150	118.895	−482.028	−305.747	9.394
1800	100.098	390.787	319.195	128.866	−481.961	−295.380	8.572
1900	100.800	396.218	323.107	138.911	−481.920	−285.016	7.836
2000	101.417	401.405	326.893	149.023	−481.908	−274.653	7.173
2100	101.962	406.366	330.560	159.192	−481.932	−264.290	6.574
2200	102.445	411.121	334.115	169.413	−481.995	−253.924	6.029
2300	102.876	415.685	337.563	179.680	−482.101	−243.555	5.531
2400	103.260	420.071	340.910	189.987	−532.512	−232.112	5.052
2500	103.605	424.294	344.161	200.330	−532.788	−219.590	4.588
2600	103.915	428.363	347.322	210.707	−533.081	−207.056	4.160
2700	104.195	432.290	350.397	221.112	−533.392	−194.510	3.763
2800	104.448	436.084	353.390	231.545	−533.721	−181.953	3.394
2900	104.678	439.754	356.305	242.001	−534.071	−169.384	3.051
3000	104.887	443.306	359.146	252.480	−534.442	−156.802	2.730
3100	105.078	446.748	361.917	262.978	−534.834	−144.208	2.430
3200	105.253	450.087	364.620	273.495	−535.248	−131.601	2.148
3300	105.413	453.328	367.259	284.028	−535.684	−118.980	1.883
3400	105.560	456.478	369.837	294.577	−536.143	−106.346	1.634
3500	105.696	459.540	372.357	305.140	−536.623	−93.698	1.398
3600	105.821	462.519	374.820	315.716	−537.127	−81.036	1.176
3700	105.937	465.420	377.230	326.304	−537.652	−68.360	.965
3800	106.044	468.246	379.588	336.903	−538.201	−55.668	.765
3900	106.143	471.002	381.897	347.512	−538.772	−42.962	.575
4000	106.236	473.691	384.158	358.131	−539.366	−30.242	.395
4100	106.322	476.315	386.374	368.759	−539.982	−17.506	.223
4200	106.402	478.878	388.546	379.395	−1020.471	2.269	−.028
4300	106.477	481.383	390.676	390.039	−1020.046	26.615	−.323
4400	106.547	483.831	392.765	400.691	−1019.646	50.951	−.605
4500	106.613	486.227	394.816	411.349	−1019.270	75.278	−.874
4600	106.674	488.570	396.828	422.013	−1018.920	99.597	−1.131
4700	106.732	490.865	398.805	432.683	−1018.596	123.909	−1.377
4800	106.787	493.113	400.746	443.359	−1018.298	148.215	−1.613
4900	106.838	495.315	402.654	454.041	−1018.027	172.515	−1.839
5000	106.886	497.474	404.529	464.727	−1017.783	196.809	−2.056
5100	106.932	499.591	406.372	475.418	−1017.567	221.099	−2.265
5200	106.975	501.668	408.185	486.113	−1017.378	245.384	−2.465
5300	107.016	503.706	409.968	496.813	−1017.218	269.667	−2.658
5400	107.054	505.707	411.722	507.516	−1017.088	293.946	−2.843
5500	107.091	507.672	413.449	518.223	−1016.987	318.223	−3.022
5600	107.125	509.601	415.149	528.934	−1016.916	342.500	−3.195
5700	107.158	511.498	416.823	539.648	−1016.877	366.774	−3.361
5800	107.189	513.362	418.471	550.366	−1016.869	391.050	−3.522
5900	107.219	515.194	420.095	561.086	−1016.893	415.322	−3.677
6000	107.247	516.997	421.695	571.810	−1016.949	439.598	−3.827

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Dihydroxyborane (B(OH)$_2$) **B$_1$H$_2$O$_2$(g)**

Borane (BH_3) **IDEAL GAS** **M_r = 13.83382 Borane (BH_3)** **$B_1H_3(g)$**

$S°(298.15\ K) = [187.88]\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = 110.5 \pm 10\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 106.7 \pm 10\ kJ\cdot mol^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}	 υ, cm^{-1}
[2384](1)	[802](1)
[1765](2)	[2976](2)

Ground State Quantum Weight: [1] $\sigma = 6$
Point Group: [D_{3h}]
Bond Distance: B–H = [1.16] Å
Bond Angle: H–B–H = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = 7.71122 \times 10^{-119}]\ g^3\cdot cm^6$

Enthalpy of Formation

$\Delta_f H°(298.15\ K)$ was calculated from appearance potentials by Fehlner and Koski.[1] For example:

$B_2H_6(g) \rightarrow BH_3^+(ion) + BH_3(g)$	13.1 eV
$BH_3^+(ion) \rightarrow BH_3(g)$	−11.4 eV
$B_2H_6(g) \rightarrow 2\ BH_3(g)$	1.7 eV

The enthalpy of formation data is summarized below.

Reaction: $B_2H_6(g) \rightarrow 2\ BH_3(g)$*

*The auxiliary $\Delta_f H°(B_2H_6,\ g,\ 298.15\ K)$ was from the JANAF table dated December 31, 1964.

Source	Method	$\Delta_f H°(0\ K)$, kcal·mol⁻¹	$\Delta_f H°(298.15\ K)$, kcal·mol⁻¹*
2	Bond energy parameters obtained by linear extrapolation from NH and CH bonds	69.9	41.7
3	Apparent equilibrium constants	55 ± 8	33
3	A recalculation by JANAF using α values and $P = 10^{-7}$ atm [α = degree of dissociation)	49 ± 8	30
4	Correlations of ionization and dissociation energies of hydrides and fluorides in relation to electronic structure	41.5	26.6
1	Appearance potentials	39.2	25.5
5	From kinetic data for the decomposition of BH_3CO	32–38	22–25
6	From calorimetric measurements of analogous compounds	28.4 ± 2	20.1
7	From electronegativities	23.9	18

Heat Capacity and Entropy

The molecular configuration, [planar, H–B–H angle 120°], was estimated by Shepp and Bauer[8] as well as by Jordan and Longuet Higgins.[2] In addition, Shepp and Bauer estimated the bond distance and the vibrational frequencies. Jordan and Longuet Higgins estimated the electronic configuration [$^1A_1'$]. The principal moments of inertia are: $I_A = I_B = 0.3378 \times 10^{-39}$ and $I_C = 0.6757 \times 10^{-39}\ g\cdot cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	S°	−[G°−H°(T_r)]/T	H°−H°(T_r)	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.129	110.478	110.478	INFINITE
100	33.268	150.652	218.682	−6.803	109.281	109.356	−57.122
200	34.135	173.880	191.116	−3.447	108.263	109.795	−28.675
250	35.114	181.598	188.466	−1.717	107.528	110.259	−23.037
298.15	36.221	187.876	187.876	0.	106.692	110.859	−19.422
300	36.266	188.100	187.876	0.067	106.658	110.885	−19.307
350	37.539	193.784	188.323	1.912	105.702	111.665	−16.665
400	38.929	198.886	189.329	3.823	104.692	112.585	−14.702
450	40.434	203.557	190.654	5.806	103.658	113.633	−13.190
500	42.038	207.900	192.164	7.868	102.622	114.797	−11.993
600	45.449	215.863	195.462	12.241	100.620	117.423	−10.223
700	48.945	223.132	198.902	16.961	98.778	120.371	−8.982
800	52.339	229.891	202.358	22.026	97.132	123.571	−8.068
900	55.510	236.241	205.774	27.421	95.683	126.964	−7.369
1000	58.397	242.242	209.123	33.119	94.413	130.510	−6.817
1100	60.980	247.931	212.395	39.090	93.296	134.175	−6.371
1200	63.268	253.337	215.583	45.305	92.305	137.935	−6.004
1300	65.282	258.483	218.687	51.735	91.412	141.775	−5.697
1400	67.049	263.387	221.706	58.353	90.594	145.680	−5.435
1500	68.599	268.067	224.642	65.137	89.832	149.642	−5.211
1600	69.959	272.538	227.497	72.066	89.108	153.653	−5.016
1700	71.153	276.816	230.273	79.123	88.409	157.708	−4.846
1800	72.206	280.914	232.973	86.292	87.722	161.804	−4.695
1900	73.135	284.843	235.601	93.560	87.040	165.939	−4.562
2000	73.959	288.616	238.158	100.916	86.353	170.109	−4.443
2100	74.690	292.242	240.647	108.349	85.655	174.314	−4.336
2200	75.342	295.732	243.072	115.851	84.942	178.552	−4.239
2300	75.925	299.094	245.435	123.415	84.209	182.824	−4.152
2400	76.447	302.337	247.739	131.034	33.193	188.196	−4.096
2500	76.917	305.467	249.986	138.703	32.331	194.673	−4.067
2600	77.341	308.492	252.178	146.416	31.473	201.183	−4.042
2700	77.725	311.419	254.319	154.170	30.615	207.727	−4.019
2800	78.073	314.252	256.409	161.960	29.756	214.302	−3.998
2900	78.389	316.997	258.451	169.783	28.894	220.908	−3.979
3000	78.677	319.659	260.447	177.637	28.026	227.544	−3.962
3100	78.941	322.244	262.399	185.518	27.153	234.209	−3.946
3200	79.183	324.754	264.309	193.424	26.271	240.902	−3.932
3300	79.404	327.194	266.177	201.354	25.380	247.624	−3.920
3400	79.608	329.567	268.007	209.305	24.480	254.372	−3.908
3500	79.796	331.878	269.799	217.275	23.568	261.146	−3.897
3600	79.970	334.128	271.555	225.263	22.644	267.947	−3.888
3700	80.131	336.321	273.276	233.269	21.707	274.774	−3.879
3800	80.280	338.460	274.963	241.289	20.756	281.627	−3.871
3900	80.418	340.547	276.618	249.324	19.791	288.504	−3.864
4000	80.547	342.585	278.242	257.372	18.811	295.407	−3.858
4100	80.667	344.575	279.836	265.433	17.816	302.334	−3.852
4200	80.779	346.521	281.400	273.506	−463.045	316.310	−3.934
4300	80.884	348.423	282.937	281.589	−462.986	334.865	−4.068
4400	80.982	350.283	284.446	289.682	−462.945	353.419	−4.196
4500	81.073	352.104	285.930	297.785	−462.924	371.973	−4.318
4600	81.160	353.887	287.388	305.897	−462.921	390.526	−4.435
4700	81.240	355.633	288.821	314.017	−462.939	409.079	−4.546
4800	81.317	357.345	290.231	322.145	−462.976	427.634	−4.654
4900	81.388	359.022	291.618	330.280	−463.033	446.188	−4.756
5000	81.456	360.667	292.983	338.422	−463.109	464.745	−4.855
5100	81.520	362.281	294.326	346.571	−463.206	483.302	−4.950
5200	81.580	363.864	295.648	354.726	−463.322	501.863	−5.041
5300	81.637	365.419	296.950	362.887	−463.457	520.425	−5.129
5400	81.691	366.945	298.232	371.053	−463.611	538.990	−5.214
5500	81.742	368.445	299.495	379.225	−463.783	557.558	−5.295
5600	81.791	369.918	300.739	387.401	−463.973	576.130	−5.374
5700	81.837	371.366	301.965	395.583	−464.181	594.705	−5.450
5800	81.880	372.790	303.174	403.769	−464.404	613.284	−5.523
5900	81.922	374.190	304.366	411.959	−464.644	631.866	−5.594
6000	81.962	375.567	305.541	420.153	−464.898	650.453	−5.663

PREVIOUS: December 1964 (1 atm) CURRENT· December 1964 (1 bar)

Boric Acid (H_3BO_3) CRYSTAL $M_r = 61.83202$ Boric Acid (H_3BO_3) $B_1H_3O_3(cr)$

$S°(298.15\ K) = 88.74 \pm 0.4\ J\cdot K^{-1}\cdot mol^{-1}$
$T_{fus} = 444.1 \pm 0.2\ K$
$T_{dcm} = [330\ K]$

$\Delta_f H°(0\ K) = -1080 \pm 0.8\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -1094 \pm 0.8\ kJ\cdot mol^{-1}$
$\Delta_{fus}H° = $ Unknown

Enthalpy of Formation

The enthalpy of formation of $\Delta_f H°(H_3BO_3, cr, 298.15\ K)$ was taken from Good and Mansson *et al.*[1] The value was derived based on the following measurements.

	$\Delta_r H°(298.15\ K)$, $kcal\cdot mol^{-1}$
$B(cr) + 0.75\ O_2(g) + 18.674\ HF\cdot 57.219\ H_2O(l) = HBF_4\cdot 14.674\ HF\cdot 58.719\ H_2O(l)$	-173.4 ± 0.2
$H_3BO_3(cr) + 18.674\ HF\cdot 55.719\ H_2O(l) = HBF_4\cdot 14.674\ HF\cdot 58.719\ H_2O(l)$	$+14.6 \pm 0.1$

The enthalpy of solution of $H_3BO_3(cr)$ in water have been measured by many investigators. Fasolino[2] obtained the value, $\Delta_r H°(298.15\ K) = 5.45 \pm 0.01\ kcal\cdot mol^{-1}$ for the reaction $H_3BO_3(cr) + 504\ H_2O(l) = H_3BO_3 504\ H_2O(sol)$ which leads to $\Delta_f H°(H_3BO_3 504\ H_2O, sol, 298.15\ K) = -256.02\ kcal\cdot mol^{-1}$. The $\Delta_r H°(298\ 15\ K)$ value is in reasonable agreement with the value reported by Smisko and Mason[3] in which the enthalpies of solution and dilution of $H_3BO_3(cr)$ were given. The enthalpies of solution of $H_3BO_3(cr)$ in water measured y other previous investigators were reviewed by Fasolino.[2]

Heat Capacity and Entropy

The low temperature (16–298.15 K) heat capacities were reported by Johnston and Kerr.[5] The heat capacities above 300 K were estimated with those of its constituent oxides. $S°(298.15\ K)$ was obtained from Johnston and Kerr using $S°(17\ K) = 0.18\ kcal\cdot mol^{-1}$.

Fusion Data

The value of T_{fus} was taken from Kracek and Morey *et al.*[6] However, $H_3BO_3(cr)$ is in a metastable state at T_{fus}. Measurements of the decomposition pressure of $H_3BO_3(cr)$ to form HBO_2(cr, II or III) and $H_2O(g)$ have been made by Menzel, Schulz and Deckert,[7] Thiel and Stiebeneck,[8] Stackelberg, Quatran and Dressel,[9] and Bezzi and Hazaki.[10] The decomposition pressures of the system $H_3BO_3(cr) = H_2O(g) + HBO_2$(cr, I), at the temperatures of 312 to 352 K, have been reported by West.[11]

Decomposition Data

The decomposition temperature (T_{dcm}) is calculated as the temperature at which the Gibbs energy change of the reaction $H_3BO_3(cr) \rightarrow HBO_2(cr) + H_2O(g)$ is zero.

Sublimation Data

The enthalpy of sublimation, $\Delta_{sub}H°(298.15\ K)$, is derived as the difference between the $\Delta_f H°(298.15\ K)$ values for $H_3BO_3(g)$ and $H_3BO_3(cr)$.

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−13.393	−1080.444	−1080.444	INFINITE
100	35.920	28.983	145.340	−11.636	−1087.566	−1049.328	548.113
200	58.743	61.128	95.458	−6.866	−1091.537	−1009.409	263.631
298.15	81.337	88 743	88.743	0.	−1093.990	−968.520	169.681
300	81.755	89.247	88.744	0.151	−1094.022	−967.741	168.499
400	100.207	115.390	92.184	9.282	−1095.069	−925.455	120.852
500	114.642	139.336	99.255	20.041	−1095.014	−883.037	92.250
600	127.194	161.372	107.795	32.146	−1094.023	−840.720	73.191
700	137.915	181.802	116.926	45.413	−1092.200	−798.636	59.595
800	147.277	200.844	126.239	59.684	−1089.646	−756.865	49.418
900	155.017	218.646	135.529	74.806	−1086.476	−715.452	41.524
1000	161.921	235.343	144.684	90.659	−1082.783	−674.421	35.228
1100	167.974	251.066	153.647	107.161	−1078.633	−633.781	30.096
1200	173.218	265.913	162.390	124.227	−1074.097	−593.538	25.836
1300	177.653	279.958	170.898	141.778	−1069.244	−553.686	22.247
1400	181.279	293.261	179.168	159.731	−1064.147	−514.218	19.186
1500	184.096	305.869	187.198	178.006	−1058.879	−475.121	16.545

PREVIOUS: September 1962   CURRENT: December 1964

Boric Acid (H_3BO_3) IDEAL GAS $M_r = 61.83202$ Boric Acid (H_3BO_3) $B_1H_3O_3(g)$

$S°(298.15\ K) = [295.237]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = Unknown$
$\Delta_fH°(298.15\ K) = -992.28 \pm 2.5\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
3250(1)	Rotation	1185(2)
1060(1)	3150(2)	Rotation
861(1)	1440(2)	Rotation
652(1)	544(2)	

Ground State Quantum Weight: 1 $\sigma = 3$
Point Group: C_{3h}
Bond Distances: B-O = [1.36] Å; O-H = [0.96] Å
Bond Angles: H-O-B = [114]°; O-B-O = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = [1.157449 \times 10^{-114}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The vapor pressures of H_3BO_3(cr), 109–140°C, were measured by Stackelberg, Quatram and Dressel.[1] Using the vapor pressures reported, the enthalpies of sublimation of H_3BO_3(cr) were evaluated to be 24.4 ± 0.6 and 24.22 $kcal{\cdot}mol^{-1}$ by the 2nd and 3rd law methods, respectively. $\Delta_fH°(H_3BO_3$, g, 298.15 K) was calculated from the $\Delta_fH°(H_3BO_3$, cr, 298.15 K) and $\Delta_{sub}H°(H_3BO_3$, cr, 298.15 K). The $\Delta_{sub}H°$(298.15 K) value adopted is the average of the 2nd and 3rd law values mentioned previously.

Heat Capacity and Entropy

The molecular structure and constants were taken from Pistorius[2] based on an x-ray diffraction study on H_3BO_3(cr) by Zachariasen.[2] The O-H bond distance was reestimated as 0.96 Å instead of 0.88 Å reported. From the existing infrared and Raman spectra data on H_3BO_3(cr) and its aqueous solution, Pistorius carried out a normal coordinate treatment by means of Wilson's F-G matrix method and calculated the fifteen fundamental frequencies for H_3BO_3(cr). For H_3BO_3(g), twelve reported frequencies were used and corrected to the average isotopic species. The three torsional frequencies, 824(1) and 209(2) cm^{-1}, were not used based on an assumption that there are three internal rotations, i.e. three OH groups, each rotates about its own B-O bond. Employing the model of having three free rotating OH tops, the value of $S°$(400 K) was evaluated statistically as 75.522 kcal mol^{-1}. The corresponding value obtained by using the 2nd law value of $\Delta_{sub}H°$(400 K), 48.39 ± 1.42 $kcal{\cdot}mol^{-1}$, for the reaction H_3BO_3(g), is 75 97 ± 1.43 $kcal{\cdot}mol^{-1}$ which is in good agreement with the $S°$(400 K) value based on a model having three free rotating groups. Thus the assumed model is adopted to evaluate the thermodynamic functions. The reduced moment of inertia for the OH top is $I_r = 1.15321 \times 10^{-40}\ g\ cm^2$. The principal moments of inertia are: $I_A = I_B = 8.3334 \times 10^{-39}$ and $I_C = 16.6669 \times 10^{-39}\ g{\cdot}cm^2$. The infrared absorption spectrum of H_3BO_3(g) was observed under conditions where one atmosphere of water vapor with a path length of approximately one meter as background, by Greene, Leroi, Randall *et al.*[4] The following fundamentals were obtained: 3220 cm^{-1} S, 1490 cm^{-1} S, 1199 cm^{-1} S, 881 cm^{-1} W, and 669 cm^{-1} W.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	12.472	0.	INFINITE	−15.356	−980.694	−980.694	INFINITE
100	46.202	237.715	345.491	−10.778	−984.995	−967.630	505.438
200	53.861	271.626	300.833	−5.841	−988.799	−948.771	247.794
250	59.585	284.250	296.280	−3.007	−990.617	−938.553	196.100
298.15	65.338	295.237	295.237	0.	−992.277	−928.373	162.647
300	65.558	295.642	295.238	0.121	−992.339	−927.976	161.575
350	71.395	306.189	296.058	3.546	−993.930	−917.121	136.873
400	76.864	316.085	297.949	7.254	−995.384	−906.048	118.318
450	81.857	325.431	300.488	11.224	−996.708	−894.800	103.866
500	86.355	334.293	303.429	15.432	−997.910	−883.411	92.289
600	94.017	350.739	309.966	24.464	−999.992	−860.309	74.897
700	100.271	365.717	316.876	34.188	−1001.711	−836.888	62.449
800	105.498	379.457	323.852	44.484	−1003.133	−813.242	53.099
900	109.953	392.147	330.744	55.262	−1004.306	−789.433	45.818
1000	113.798	403.935	337.481	66.454	−1005.275	−765.505	39.986
1100	117.137	414.942	344.028	78.005	−1006.076	−741.487	35.210
1200	120.047	425.262	350.372	89.868	−1006.743	−717.404	31.228
1300	122.589	434.973	356.510	102.002	−1007.306	−693.269	27.856
1400	124.814	444.141	362.445	114.375	−1007.789	−669.093	24.964
1500	126.764	452.821	368.183	126.956	−1008.217	−644.886	22.457
1600	128.478	461.058	373.733	139.720	−1008.607	−620.651	20.262
1700	129.988	468.893	379.102	152.645	−1008.976	−596.392	18.325
1800	131.321	476.361	384.299	165.711	−1009.338	−572.113	16.602
1900	132.501	483 494	389.334	178.904	−1009.706	−547.812	15.060
2000	133.550	490.317	394.214	192.207	−1010.089	−523.492	13.672
2100	134.484	496.856	398.947	205.610	−1010.495	−499.152	12.416
2200	135.319	503.132	403.541	219.101	−1010.932	−474.792	11.273
2300	136.067	509.164	408.003	232.671	−1011.405	−450.412	10.229
2400	136.740	514.969	412.340	246.312	−1062.178	−424.942	9.249
2500	137.346	520.564	416.557	260.017	−1062.816	−398.377	8.324
2600	137.893	525.962	420.662	273.779	−1063.470	−371.787	7.469
2700	138.390	531.175	424.659	287.594	−1064.142	−345.170	6.678
2800	138.841	536.216	428.554	301.456	−1064.836	−318.529	5.942
2900	139.251	541.096	432.351	315.360	−1065.553	−291.863	5.257
3000	139.626	545.823	436.055	329.305	−1066.296	−265.171	4.617
3100	139.970	550.407	439.670	343.285	−1067.064	−238.454	4.018
3200	140.284	554.856	443.200	357.298	−1067.860	−211.713	3.456
3300	140.574	559.177	446.650	371.341	−1068.683	−184.946	2.927
3400	140.840	563.378	450.021	385.412	−1069.535	−158.153	2.430
3500	141.086	567.464	453.319	399.508	−1070.417	−131.335	1.960
3600	141.313	571.442	456.545	413.628	−1071.328	−104.491	1.516
3700	141.524	575.316	459.703	427.770	−1072.269	−77.622	1.096
3800	141.719	579.093	462.795	441.932	−1073.241	−50.726	0.697
3900	141.901	582.777	465.825	456.114	−1074.243	−23.804	0.319
4000	142.070	586.372	468.794	470.312	−1075.276	3.142	−0.041
4100	142.227	589.882	471.704	484.527	−1076.340	30.116	−0.384
4200	142.374	593.311	474.559	498.757	−1557.285	64.140	−0.798
4300	142.512	596.663	477.360	513.002	−1557.325	102.747	−1.248
4400	142.641	599.940	480.109	527.259	−1557.399	141.353	−1.678
4500	142.762	603.147	482.807	541.530	−1557.507	179.961	−2.089
4600	142.875	606.286	485.458	555.812	−1557.650	218.573	−2.482
4700	142 982	609.360	488.061	570.104	−1557.828	257.189	−2.858
4800	143.082	612.371	490.620	584.408	−1558.042	295.809	−3.219
4900	143.176	615.323	493.135	598.721	−1558.293	334.434	−3.565
5000	143.266	618.216	495.608	613.043	−1558.581	373.064	−3.897
5100	143.350	621.054	498.040	627.374	−1558.907	411.700	−4.217
5200	143.429	623.838	500.432	641.713	−1559.272	450.342	−4.524
5300	143.505	626.571	502.786	656.059	−1559.675	488.993	−4.819
5400	143.576	629.254	505.104	670.413	−1560.119	527.651	−5.104
5500	143.643	631.889	507.385	684.774	−1560.604	566.317	−5.378
5600	143.707	634.478	509.631	699.142	−1561.130	604.994	−5.643
5700	143.768	637.022	511.844	713.516	−1561.698	643.679	−5.899
5800	143.826	639.523	514.024	727.895	−1562.309	682.377	−6.145
5900	143.881	641.982	516.172	742.281	−1562.964	721.081	−6.384
6000	143.934	644.401	518.289	756.672	−1563.664	759.801	−6.615

PREVIOUS. December 1964 (1 atm) CURRENT. December 1964 (1 bar)

Boric Acid (H_3BO_3) $B_1H_3O_3(g)$

Potassium Tetrahydroborate (KBH$_4$) CRYSTAL M_r = 53.94006 Potassium Tetrahydroborate (KBH$_4$) B$_1$H$_4$K$_1$(cr)

$S°(298.15\ \mathrm{K}) = 106.61\ \mathrm{J{\cdot}K^{-1}{\cdot}mol^{-1}}$

$\Delta_f H°(0\ \mathrm{K}) = -218\ 19 \pm 2\ 30\ \mathrm{kJ{\cdot}mol^{-1}}$
$\Delta_f H°(298.15\ \mathrm{K}) = -226.90 \pm 2.30\ \mathrm{kJ{\cdot}mol^{-1}}$

Enthalpy of Formation

The enthalpy of reaction of KBH$_4$(cr) with hydrochloric acid has been measured by solution calorimetry and reported by Johnson, Schumm, Wilson, and Prosen.[4]

$$\mathrm{KBH_4(cr) + HCl(g) + 3H_2O(l) \rightarrow KCl(cr) + H_3BO_3(cr) + 4H_2(g)}\ \Delta_r H° = -84.62 \pm 0.44\ \mathrm{kcal{\cdot}mol^{-1}}$$

The $\Delta_f H(298.15\ \mathrm{K})$ values for HCl(g) and H$_3$BO$_3$(cr) were obtained from the JANAF Tables. The $\Delta_f H°(298.15\ \mathrm{K})$ value for KCl(cr) was calculated from $\Delta_f H°(\mathrm{K^+}, \mathrm{aq}, \infty, 298.\ 15\ \mathrm{K}) = -60.32\ \mathrm{kcal{\cdot}mol^{-1}}$, $\Delta_f H°(\mathrm{Cl^-}, \mathrm{aq}, \infty, 298.15\ \mathrm{K}) = -39.952\ \mathrm{kcal{\cdot}mol^{-1}}$ and $\Delta_{dil} H° = 4.12\ \mathrm{kcal{\cdot}mol^{-1}}$ obtained by Evans.[4] $\Delta_f H°(298.15\ \mathrm{K})$ for H$_2$O(l) was obtained from Evans.[4] Unpublished data of The Dow Chemical Company Thermal laboratory give a value of $\Delta_f H°(298.15\ \mathrm{K}) = -55.0 \pm 1\ 0\ \mathrm{kcal{\cdot}mol^{-1}}$ by solution calorimetry.

Heat Capacity and Entropy

C_p and $S°$ at temperatures below 298.15 K were reported by Furukawa, Reilly, and Henning.[2] The values of C_p in the range from 298.15 to 700 K were obtained from Douglas and Harman.[3] These two sets of C_p data were plotted and joined smoothly at 298.15 K. The values of C_p above 700 K are estimated by graphical extrapolation.

Decomposition Data

The temperature of decomposition (into constituent elements) was estimated to be 770 K, according to a report by Douglas and Harman.[3]

References

[1] W. H. Johnson, R. H. Schumm, I. H. Wilson, and E. J. Prosen, J. Res. Nat. Bur. Stand. 65A, 97 (1961).
[2] G. T. Furukawa, M L. Reilly, and J. M. Henning, J. Res. Nat. Bur. Stand. 68A, 651 (1964).
[3] T. B. Douglas and A. W. Harman, J. Res. Nat. Bur. Stand. 60, 117 (1958).
[4] W. H. Evans, U. S. Nat. Bur. Stand. Report 8504, Appendix III, 164 (1964).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−16.523	−218.190	−218.190	INFINITE
100	43.388	32.560	176.531	−14.397	−223.820	−203.339	106.213
200	73.580	72.530	114.809	−8.456	−226.193	−181.752	47 469
298.15	96.571	106.608	106.608	0.	−226.898	−159.738	27.986
300	96.734	107.206	106.610	0.179	−226.902	−159.322	27.740
400	100.918	135 797	110.480	10.127	−229.606	−136.305	17.800
500	102.131	158.434	117.887	20.273	−230.144	−112.920	11.797
600	106.033	177.333	126.258	30.645	−230.651	−89.424	7.785
700	115.227	194.306	134.780	41.668	−230.655	−65.874	4.916
800	118.407	209.909	143.213	53.356	−230.132	−42.368	2.766
900	120.625	223.988	151.419	65.312	−229.490	−18.935	1.099
1000	122.340	236.790	159.326	77.464	−228.820	4.424	−0.231
1100	123.386	248.501	166.908	89.752	−307.159	32.327	−1.535
1200	124.265	259.276	174.162	102.136	−305.599	63.120	−2.748
1300	124.919	269.248	181.098	114.596	−304.101	93.786	−3.768
1400	125.520	278.528	187.730	127.118	−302.676	124.339	−4.639
1500	126.060	287.207	194.075	139.697	−301.326	154.792	−5.390
1600	126.566	295.359	200.153	152.329	−300.054	185.158	−6 045
1700	127.037	303.046	205.982	165.009	−298.859	215.447	−6.620
1800	127.473	310.320	211.578	177.735	−297.741	245.667	−7.129
1900	127.873	317.223	216.958	190.503	−296.700	275.828	−7.583
2000	128.240	323.791	222.137	203.309	−295.735	305.936	−7.990

PREVIOUS: March 1963 CURRENT: December 1964

Lithium Tetrahydroborate ($LiBH_4$) CRYSTAL $M_r = 21.78276$ Lithium Tetrahydroborate ($LiBH_4$) $B_1H_4Li_1(cr)$

$\Delta_fH°(0\ K) = -180.391 \pm 0.21\ kJ \cdot mol^{-1}$
$\Delta_fH°(298.15\ K) = -190.464 \pm 0.21\ kJ \cdot mol^{-1}$
$\Delta_{fus}H° =$ Unknown

$S°(298.15\ K) = 75.82\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{fus} = [750]\ K$

Enthalpy of Formation

The enthalpy of formation of LiBH4(cr) was calculated from the solution calorimetry of Davis, Mason and Stegeman.[1] The enthalpies of reaction were measured for the following reactions:

$LiBH_4(cr) + 1.25(HCl \cdot 200\ H_2O) + 3\ H_2O(l) \rightarrow (NaCl + H_3BO_3 + 0.25\ HCl)247\ H_2O + 4\ H_2(g)$ $\Delta H_1(298.15\ K) = -72.14$ kcal mol^{-1}
$LiCl \cdot 60\ H_2O + H_3BO_3 \cdot 60\ H_2O + 0.25(HCl \cdot 506\ H_2O) \rightarrow (LiCl + H_3BO_3 + 0.25\ HCl) \cdot 247\ H_2O$ $\Delta H_2(298.15\ K) = 0.00$ kcal mol^{-1} (assumed)
$H_3BO_3 \cdot 60\ H_2O + \infty\ H_2O \rightarrow H_3BO_3 \cdot \infty\ H_2O$ $^*\Delta H_3(298.15\ K) = 0.200$ kcal mol^{-1}

The summation of the above reactions yields:

$LiBH_4(cr) + 1.25(HCl \cdot 200\ H_2O) + 3\ H_2O(l) + \infty\ H_2O \rightarrow LiCl \cdot 60\ H_2O + H_3BO_3 \cdot \infty\ H_2O + 0.25(HCl \cdot 508\ H_2O) + 4\ H_2(g)$ $\Delta H(298.15\ K) = -71.94$

*This $\Delta_fH°(298.15\ K)$ value was obtained from J. Smisko and L. S. Mason loc. cit.

The enthalpy of formation of lithium borohydride crystal was calculated to be −45.522 kcal mol^{-1} with the following auxiliary data:

Compound	$\Delta_fH°(298.15\ K)$	Source
HCl (508 H_2O)	−39.815	HCl(g) JANAF; *dilution data from NBS Rept. 8504, 1 July 1964* Appendix III by W. H. Evans
HCl (200 H_2O)	−39.696	HCl(g) JANAF; dilution data fromW. H. Evans, loc. cit.
LiCl (60 H_2O)	−106.023	Li^+ see NaBH4 table; Cl^- and dilution data, W. H. Evans, loc. cit.
$H_3BO_3(\infty H_2O)$	−256.05	JANAF $H_3BO_3(cr)$ and dilution data from J. Smisko and L. S. Mason, J. Am. Chem. Soc. **72**, 3679 (1950).

Heat Capacity and Entropy

The low temperature heat capacities, 15.72–302.88 K, were obtained from the measurements by Hallett and Johnston.[2] The C_p values above 298.15 K were estimated by comparison with the C_p's for $NaBH_4$.

The entropy was based on $S°(15\ K,\ extrap) = 0.0874\ cal \cdot K^{-1} \cdot mol^{-1}$ reported by Hallett and Johnston.[2]

Fusion Data

T_{fus} was estimated by comparison with the T_{fus} for $NaBH_4$.

References

[1] W. D. Davis, L. S. Mason and G. Stegeman, J. Am. Chem. Soc. **71**, 2775 (1949).
[2] N. C. Hallett and H. L. Johnston, J. Am. Chem. Soc. **75**, 1496 (1953).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−12.697	−180.391	−180.391	INFINITE
90	30.019	17.086	132.466	−11.538	−185.749	−166.547	86.995
200	59.575	47.990	82.538	−6.910	−188.682	−146.067	38.149
298.15	82.539	75.815	75.815	0.	−190.464	−124.733	21.853
300	82.989	76.326	75.817	0.153	−190.484	−124.325	21.647
400	91.002	101.384	79.181	8.881	−191.531	−102.115	13.335
500	98.282	122.480	85.783	18.349	−195.573	−79.333	8.288
600	105.144	141.037	93.475	28.537	−196.207	−56.016	4.877
700	109.914	157.625	101.476	39.304	−196.396	−32.631	2.435
800	113.052	172.527	109.442	50.468	−196.317	−9.239	0.603
900	114.349	185.920	117.209	61.840	−196.167	14.136	−0.820
1000	115.353	198.020	124.695	73.325	−196.037	37.496	−1.959
1100	116.392	209.064	131.870	84.913	−195.938	60.844	−2.889
1200	117.319	219.232	138.732	96.600	−195.873	84.185	−3.664
1300	118.019	228.650	145.291	108.367	−195.861	107.522	−4.320
1400	118.684	237.421	151.562	120.203	−195.910	130.861	−4.882
1500	119.316	245.631	157.563	132.103	−196.017	154.205	−5.370
1600	119.913	253.351	163.311	144.065	−196.184	177.558	−5.797
1700	120.477	260.638	168.823	156.084	−341.644	208.100	−6.394
1800	121.007	267.539	174.118	168.159	−341.173	240.424	−6.977
1900	121.502	274.095	179.209	180.285	−340.766	272.723	−7.498
2000	121.964	280.339	184.110	192.458	−340.424	305.003	−7.966

PREVIOUS: March 1963 CURRENT: December 1964

Sodium Tetrahydroborate ($NaBH_4$) CRYSTAL M_r = 37.83153 Sodium Tetrahydroborate ($NaBH_4$) $B_1H_4Na_1(cr)$

$S°(298.15\ K) = 101.39\ J·K^{-1}·mol^{-1}$
$T_{trs} = 189.9\ K$
$T_{fus} = 770\ K$

$\Delta_fH°(0\ K) = -183.3 \pm 0.39\ kJ·mol^{-1}$
$\Delta_fH°(298.15\ K) = -191.84 \pm 0.39\ kJ·mol^{-1}$
$\Delta_{trs}H° = 0.999\ kJ·mol^{-1}$
$\Delta_{fus}H°$ = Unknown

Enthalpy of Formation

The enthalpy of formation is calculated from the solution calorimetry of Davis, Mason and Stegeman.[1] The enthalpies of reaction and mixing were measured for the following reactions:

$NaBH_4 + 1.25(HCl·200H_2O) \rightarrow (NaCl + H_3BO_3 + 0\ 25HCl)·247H_2O + 4H_2$ $\Delta_rH = -63.880\ kcal·mol^{-1}$
$NaCl·60H_2O + H_3BO_3·60H_2O \rightarrow (NaCl + H_3BO_3)·120H_2O$ $\Delta_rH = -0.026\ kcal·mol^{-1}$
$NaCl + (H_3BO_3)·120H_2O + 0.25(HCl·508H_2O) \rightarrow (NaCl + H_3BO_3 + 0.25HCl)·247H_2O$ $\Delta_rH = +0.083\ kcal·mol^{-1}$
$H_3BO_3·60H_2O + \infty H_2O \rightarrow H_3BO_3\infty H_2O$ $\Delta_rH = +0.068\ kcal·mol^{-1}$
The summation of the above equations yields:
$NaBH_4(cr) + 1.25(HCl·200H_2O) + 3H_2O(1) + \infty H_2O \rightarrow NaCl\ 60H_2O + H_3BO_3\infty H_2O + 0.25(HCl·508H_2O) + 4H_2(g)$
$\Delta_rH = -63.869\ kcal·mol^{-1}$

The $\Delta_fH(298.15\ K)$ values for HCl were obtained from JANAF value[5] for HCl(g) and enthalpy of dilution data of Evans.[6] The $\Delta_fH(298.15\ K)$ for $H_2O(1)$ value was obtained from Evans.[6] The $\Delta_fH(298.15\ K)$ value for NaCl was obtained from JANAF value[5] of NaCl(cr) together with dilution data from Evans.[6] The $\Delta_fH(298.15\ K)$ value for H_3BO_3 was obtained from JANAF value[5] for $H_3BO_3(cr)$ together with dilution data of Smisko and Mason.[2]

Heat Capacity And Entropy

The low temperature heat capacity (15.76–301.26 K) was obtained from Johnston and Hallett.[3] In the area of transition (169–193.5 K) the average $\Delta_{trs}H = 635.3\ cal·mol^{-1}$ and the average $\Delta_{trs}S = 3.35\ cal·K^{-1}·mol^{-1}$ were adopted from Johnston and Hallett.[3] Using the present base line these ΔH and ΔS values yield a enthalpy of transition of $0.2388\ kcal·mol^{-1}$. The low temperature heat capacity was fitted with the smoothed enthalpy capacity data (298.15–700 K) of Douglas and Harman.[4] The heat capacity above 700 K was extrapolated from the plot of both sets of data.

Transition Data

The temperature and heat of transition were obtained from Johnston and Hallett.[3]

Fusion Data

The fusion data was obtained from Douglas and Harman.[4]

References

[1] W D. Davis, L. S. Mason, and G. Stegeman, J. Amer. Chem. Soc. 71, 2775 (1949).
[2] J. Smisko and L. S. Mason, J Am. Chem. Soc. 72, 3679 (1950).
[3] H. L. Johnston and N. C. Hallett, J. Amer. Chem. Soc. 75, 1467 (1953).
[4] T. B. douglas and A. W. Harman, J. Res. Nat. Bur. Stand. 60, 117 (1958).
[5] JANAF Thermochemical Tables: HCl(g), 9–30–64, NaCl(cr), 9–30–64; $H_3BO_3(cr)$, 12–31–64.
[6] W. H. Evans, U.S. Nat. Bur. Stand., Report 8504, Appendix III, (1964).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	$\log K_f$
0	0.	0.	INFINITE	−16.288	−183.530	−183.530	INFINITE
100	40.158	26.309	172.080	−14.577	−189.180	−169.254	88.409
200	71.446	69.772	108.872	−7.820	−190.599	−148.166	38.697
298.15	86.483	101.387	101.387	0.	−191.836	−127.060	22.260
300	86 642	101.922	101.388	0.160	−191.856	−126.658	22.053
400	94.558	127.958	104.885	9.229	−195.583	−104.556	13.654
500	101.797	149.845	111.743	19.051	−196.439	−81.690	8.534
600	108.617	169.013	119.722	29.575	−196.771	−58.700	5.110
700	115.269	186.259	128.014	40.771	−196.558	−35.697	2.664
800	120.248	201.987	136.293	52.555	−195.870	−12.759	0.833
900	124.265	216.397	144.404	64.793	−194.851	10.071	−0.585
1000	127.445	229.654	152.275	77.379	−193.622	32.776	−1.712
1100	130.039	241.923	159.874	90.253	−192.264	55.351	−2.628
1200	131.754	253.314	167.192	103.346	−287.627	80.239	−3.493
1300	132.675	263.902	174.229	116.575	−285.360	110.802	−4.452
1400	133.135	273.754	180.990	129.869	−283.162	141.193	−5.268
1500	133.302	282.945	187.485	143.191	−281.069	171.431	−5.970
1600	133.428	291.553	193.723	156.528	−279.090	201.532	−6.579
1700	133.511	299.644	199.718	169.875	−277.224	231.513	−7.114
1800	133.553	307.276	205.483	183.228	−275.473	261.388	−7.585
1900	133.679	314.500	211.033	196.589	−273.829	291.168	−8.005
2000	133.888	321.362	216.379	209.966	−272.279	320.864	−8.380

PREVIOUS. December 1960 CURRENT: December 1964

Iodoborane (BI) IDEAL GAS $M_r = 137.7145$ Iodoborane (BI) $B_1I_1(g)$

$S°(298.15\ K) = [232.75]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = [304 \pm 42]\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = [305 \pm 42]\ kJ{\cdot}mol^{-1}$

Electronic Level and Quantum Weight State	ϵ_i, cm^{-1}	g_i
$[^1\Sigma^+]$	0	[1]

$\omega_e = [600]\ cm^{-1}$ $\omega_e x_e = [3.04]\ cm^{-1}$ $\sigma = 1$
$B_e = [0.3912]\ cm^{-1}$ $\alpha_e = [0.0027]\ cm^{-1}$ $r_e = [2.08]$ Å

Enthalpy of Formation

The ratio, $D_0^\circ(BF)\ /\ (\Delta_a H°(BF_3, g, 0\ K)/3) = 1.177$, was applied to BI_3 giving $D_0^\circ(BI) = 84.4\ kcal{\cdot}mol^{-1}$ and $\Delta_f H°(298.15\ K) = 73 \pm 10\ kcal{\cdot}mol^{-1}$

Heat Capacity and Entropy

The bond length was first estimated by comparison with the ratio of the bond lengths in the other boron trihalides and monohalides. The vibrational frequency was then calculated using Guggenheimer's Relation[1] which was checked using BBr_3 and shown to give an excellent fit. The quantity $x_e\mu^{1/2}$, where μ is the reduced mass, has been shown to be for similar molecules and its value was transferred from BBr to give x_e and $\omega_e x_e$ for BI. α_e was then calculated using the Morse potential function and B_e was determined from the bond length. The ground state configuration was assumed to be the same as that in BBr.

Reference

[1] E. A. Guggenheimer, *Proc. Phys. Soc. (London)* 58, 456 (1946).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.113	304.132	304.132	INFINITE
100	29.230	199.010	261.032	−6.202	305.494	288.673	−150.787
200	31.317	219.800	235.754	−3.191	305.706	271.726	−70.967
250	32.566	226.926	233.297	−1.593	305.619	263.238	−55.001
298.15	33.558	232.750	232.750	0.	305.432	255.091	−44.691
300	33.592	232.958	232.751	0.062	305.423	254.779	−44.361
350	34.389	238.198	233.163	1.763	305.090	246.362	−36.767
400	35.002	242.832	234.087	3.498	296.677	238.274	−31.115
450	35.475	246.983	235.294	5.260	295.595	231.038	−26.818
500	35.846	250.741	236.654	7.044	274.394	225.825	−23.592
600	36.381	257.327	239.566	10.657	274.149	216.132	−18.816
700	36.742	262.964	242.515	14.314	273.767	206.491	−15.409
800	37.001	267.888	245.386	18.002	273.282	196.912	−12.857
900	37.197	272.258	248.133	21.712	272.716	187.399	−10.876
1000	37.351	276.186	250.746	25.440	272.080	177.953	−9.295
1100	37.478	279.752	253.223	29.182	271.384	168.573	−8.005
1200	37.586	283.017	255.572	32.935	270.633	159.259	−6.932
1300	37.679	286.030	257.800	36.698	269.826	150.011	−6.028
1400	37.763	288.825	259.918	40.471	268.965	140.826	−5.254
1500	37.839	291.433	261.933	44.251	268.048	131.705	−4.586
1600	37.909	293.877	263.854	48.038	267.070	122.647	−4.004
1700	37.975	296.178	265.688	51.832	266.030	113.652	−3.492
1800	38.037	298.350	267.443	55.633	264.926	104.720	−3.039
1900	38.096	300.408	269.124	59.440	263.756	95.851	−2.635
2000	38.153	302.364	270.738	63.252	262.521	87.046	−2.273
2100	38.208	304.227	272.288	67.070	261.222	78.304	−1.948
2200	38.262	306.005	273.781	70.894	259.863	69.625	−1.653
2300	38.314	307.707	275.219	74.723	258.449	61.009	−1.386
2400	38.365	309.339	276.607	78.557	206.724	53.525	−1.165
2500	38.415	310.906	277.948	82.396	205.136	47.174	−0.986
2600	38.465	312.414	279.245	86.240	203.542	40.888	−0.821
2700	38.514	313.866	280.500	90.089	201.948	34.662	−0.671
2800	38.562	315.268	281.717	93.942	200.358	28.495	−0.532
2900	38.609	316.622	282.897	97.801	198.780	22.385	−0.403
3000	38.657	317.932	284.044	101.664	197.216	16.329	−0.284
3100	38.704	319.200	285.157	105.532	195.673	10.325	−0.174
3200	38.750	320.429	286.240	109.405	194.152	4.370	−0.071
3300	38.797	321.623	287.295	113.282	192.658	−1.537	0.024
3400	38.843	322.781	288.321	117.164	191.192	−7.400	0.114
3500	38.888	323.908	289.322	121.051	189.758	−13.220	0.197
3600	38.934	325.004	290.298	124.942	188.355	−18.999	0.276
3700	38.979	326.072	291.251	128.838	186.986	−24.740	0.349
3800	39.025	327.112	292.181	132.738	185.650	−30.444	0.418
3900	39.070	328.126	293.089	136.642	184.349	−36.114	0.484
4000	39.115	329.116	293.978	140.552	183.082	−41.751	0.545
4100	39.160	330.082	294.847	144.465	181.849	−47.356	0.603
4200	39.204	331.026	295.697	148.384	−299.200	−45.908	0.571
4300	39.249	331.949	296.529	152.306	−299.279	−39.876	0.484
4400	39.293	332.852	297.345	156.233	−299.328	−33.843	0.402
4500	39.338	333.736	298.143	160.165	−299.346	−27.809	0.323
4600	39.382	334.601	298.927	164.101	−299.336	−21.775	0.247
4700	39.427	335.448	299.695	168.041	−299.298	−15.741	0.175
4800	39.471	336.279	300.448	171.986	−299.233	−9.708	0.106
4900	39.515	337.093	301.188	175.936	−299.143	−3.678	0.039
5000	39.559	337.892	301.914	179.889	−299.029	2.351	−0.025
5100	39.603	338.676	302.627	183.847	−298.892	8.377	−0.086
5200	39.647	339.445	303.328	187.810	−298.733	14.401	−0.145
5300	39.691	340.201	304.016	191.777	−298.553	20.421	−0.201
5400	39.735	340.943	304.693	195.748	−298.354	26.437	−0.256
5500	39.779	341.672	305.359	199.724	−298.136	32.450	−0.308
5600	39.823	342.390	306.014	203.704	−297.901	38.459	−0.359
5700	39.867	343.095	306.658	207.689	−297.650	44.463	−0.407
5800	39.911	343.789	307.293	211.677	−297.383	50.463	−0.454
5900	39.955	344.471	307.917	215.671	−297.103	56.457	−0.500
6000	39.999	345.143	308.532	219.668	−296.810	62.448	−0.544

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Diiodoborane (BI$_2$) **IDEAL GAS** **M_r = 264.6190** **Diiodoborane (BI$_2$)** **B$_1$I$_2$(g)**

$S°(298.15\ K) = [309.56]\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = [245 \pm 63]\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [243 \pm 63]\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[550](1)
[110](1)
[770](1)

Ground State Quantum Weight: [2] $\sigma = 2$
Point Group: [C$_{2v}$]
Bond Distance: B–I = [2.06] Å
Bond Angle: I–B–I = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = [3.331449 \times 10^{-113}]\ g^3 \cdot cm^6$

Enthalpy of Formation

The enthalpy of formation was estimated by analogy with BF$_3$, specifically the ratio $\Delta_r H°(BX_3 \rightarrow BX_2 + X) / \Delta_r H°(BX_3 \rightarrow B + 3X)$ was taken as 0.347.

Heat Capacity and Entropy

The vibrational frequencies were obtained from force constants transferred from the trihalide given by Herzberg.[1] The bond length was taken between those of the mono and trihalide and the angle was estimated to be the same as that in the trihalides. The ground state quantum weight was taken as two on account of the one unpaired electron.

The principal moments of inertia are: $I_A = 1.8266 \times 10^{-39}$, $I_B = 134.1401 \times 10^{-39}$, and $I_C = 135.9667 \times 10^{-39}\ g \cdot cm^2$.

Reference

[1] G. Herzberg, "Infrared and Raman Spectra of Polyatomic Molecules," D. Van Nostrand, Inc., (1945).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−12.522	244.562	244.562	INFINITE
100	40.240	261.642	350.181	−8.854	245.156	225.122	−117.592
200	44.749	290.842	313.919	−4.615	244.129	205.436	−53.654
250	47.122	301.087	310.357	−2.318	243.428	195.842	−40.919
298.15	49.083	309.560	309.560	0.	242.672	186.744	−32.717
300	49.151	309.864	309.561	0.091	242.641	186.397	−32.455
350	50.786	317.568	310.165	2.591	241.702	177.094	−26.430
400	52.076	324.437	311.528	5.164	224.713	168.481	−22.001
450	53.089	330.632	313.312	7.794	222.482	161.585	−18.756
500	53.889	336.268	315.330	10.469	180.091	158.739	−16.583
600	55.037	346.202	319.670	15.920	179.806	154.494	−13.450
700	55.796	354.747	324.085	21.464	179.428	150.304	−11.216
800	56.317	362.234	328.395	27.071	178.973	146.173	−9.544
900	56.689	368.890	332.532	32.722	178.452	142.104	−8.247
1000	56.962	374.877	336.472	38.405	177.871	138.096	−7.213
1100	57.168	380.316	340.214	44.112	177.233	134.149	−6.370
1200	57.328	385.298	343.767	49.838	176.537	130.262	−5.670
1300	57.453	389.892	347.140	55.577	175.779	126.436	−5.080
1400	57.554	394.153	350.348	61.327	174.952	122.671	−4.577
1500	57.635	398.127	353.402	67.087	174.050	118.968	−4.143
1600	57.702	401.849	356.315	72.854	173.064	115.327	−3.765
1700	57.758	405.349	359.098	78.627	171.985	111.751	−3.434
1800	57.805	408.651	361.760	84.405	170.808	108.242	−3.141
1900	57.845	411.778	364.311	90.188	169.529	104.800	−2.881
2000	57.880	414.746	366.759	95.974	168.147	101.429	−2.649
2100	57.909	417.571	369.112	101.764	166.666	98.129	−2.441
2200	57.935	420.265	371.376	107.556	165.091	94.902	−2.253
2300	57.957	422.841	373.558	113.350	163.429	91.748	−2.084
2400	57.977	425.308	375.663	119.147	111.432	89.737	−1.953
2500	57.994	427.675	377.697	124.946	109.552	88.872	−1.857
2600	58.010	429.950	379.663	130.746	107.651	88.082	−1.770
2700	58.024	432.140	381.566	136.548	105.741	87.366	−1.690
2800	58.036	434.250	383.410	142.351	103.833	86.720	−1.618
2900	58.047	436.287	385.199	148.155	101.937	86.143	−1.552
3000	58.057	438.255	386.935	153.960	100.064	85.630	−1.491
3100	58.066	440.159	388.621	159.766	98.222	85.179	−1.435
3200	58.074	442.002	390.261	165.573	96.418	84.787	−1.384
3300	58.082	443.789	391.856	171.381	94.657	84.451	−1.337
3400	58.089	445.523	393.409	177.190	92.946	84.168	−1.293
3500	58.095	447.207	394.922	182.999	91.288	83.934	−1.253
3600	58.101	448.844	396.397	188.809	89.685	83.747	−1.215
3700	58.106	450.436	397.836	194.619	88.140	83.603	−1.180
3800	58.111	451.986	399.241	200.430	86.655	83.501	−1.148
3900	58.116	453.495	400.613	206.241	85.229	83.437	−1.118
4000	58.120	454.967	401.953	212.053	83.863	83.408	−1.089
4100	58.124	456.402	403.264	217.865	82.556	83.413	−1.063
4200	58.127	457.802	404.546	223.678	−398.541	90.473	−1.125
4300	58.131	459.170	405.800	229.490	−398.644	102.117	−1.240
4400	58.134	460.507	407.029	235.304	−398.692	113.764	−1.351
4500	58.137	461.813	408.232	241.117	−398.686	125.411	−1.456
4600	58.139	463.091	409.410	246.931	−398.630	137.057	−1.556
4700	58.142	464.341	410.566	252.745	−398.524	148.701	−1.653
4800	58.144	465.565	411.699	258.559	−398.371	160.343	−1.745
4900	58.147	466.764	412.811	264.374	−398.173	171.981	−1.833
5000	58.149	467.939	413.901	270.189	−397.931	183.614	−1.918
5100	58.151	469.091	414.972	276.004	−397.648	195.242	−2.000
5200	58.153	470.220	416.024	281.819	−397.326	206.864	−2.078
5300	58.155	471.328	417.057	287.634	−396.967	218.480	−2.153
5400	58.156	472.415	418.072	293.450	−396.572	230.088	−2.226
5500	58.158	473.482	419.070	299.266	−396.144	241.689	−2.295
5600	58.159	474.530	420.051	305.081	−395.685	253.282	−2.363
5700	58.161	475.559	421.016	310.897	−395.196	264.867	−2.427
5800	58.162	476.571	421.965	316.714	−394.680	276.442	−2.490
5900	58.164	477.565	422.899	322.530	−394.137	288.009	−2.550
6000	58.165	478.542	423.818	328.346	−393.570	299.566	−2.608

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Diiodoborane (BI$_2$) **B$_1$I$_2$(g)**

$S°(298.15\ K)$ = [348.72] J·K^{-1}·mol^{-1}

$\Delta_fH°(0\ K)$ = 75 ± 50 kJ·mol^{-1}
$\Delta_fH°(298.15\ K)$ = 71 ± 50 kJ·mol^{-1}

Vibrational Frequencies and Degeneracies ν, cm^{-1}
190(1)
339(1)
710(2)
100(2)

Ground State Quantum Weight: [1]
Point Group: D_{3h}
Bond Distance: B–I = [2.03 ± 0.03] Å
Bond Angle: I–B–I = [120]°
Product of the Moments of Inertia: $I_AI_BI_C$ = [4.420581 × 10^{-111}] g^3·cm^6

$\sigma = 6$

Enthalpy of Formation

Koski *et al.*[2] measured the appearance potential of the B^+ ion from BI_3. Assuming the reaction $BI_3 + e^- \rightarrow B^+ + 3I + 2e^-$, one can calculate the enthalpy of atomization of BI_3 as 8.31 ± 0.5 eV. The analogous reaction for BBr_3 can be checked independently and shows the process to be valid. This value leads to $\Delta_fH°(298.15\ K)$ = 17.0 ± 12 kcal·mol^{-1} if the process is assumed to occur at 298.15 K.

Heat Capacity and Entropy

Vibrational frequencies were taken from Wentink and Tiensuu,[1] modified according to the natural abundance of boron. The B–I distance was estimated by Koski *et al.*[2] and the angle was estimated by analogy with the other boron trihalides. The three principal moments of inertia are: $I_A = I_B$ = 130.2616 × 10^{-39}, and I_C = 260.5232 × 10^{-39} g·cm^2.

References

[1] T. Wentink and V. H. Tiensuu, J. Chem. Phys. 28, 826 (1958).
[2] W. S. Koski, J. J. Kaufman, and C. F. Pochuki, J. Am Chem. Soc. 81, 1326 (1959).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	-16.839	75.300	75.300	INFINITE
100	53.503	281.071	406.863	-12.579	74.961	56.033	-29.269
200	64.157	321.770	355.004	-6.647	73.162	37.779	-9.867
250	67.907	336.504	349.871	-3.342	72.154	29.048	-6.069
298.15	70.787	348.721	348.721	0.	71.128	20.838	-3.651
300	70.884	349.159	348.723	0.131	71.087	20.526	-3.574
350	73.197	360.268	349.595	3.736	69.846	12.193	-1.820
400	74.982	370.163	351.559	7.442	44.578	4.867	-0.636
450	76.365	379.078	354.129	11.227	41.485	0.089	-0.010
500	77.445	387.182	357.035	15.073	-21.816	1.355	-0.142
600	78.984	401.449	363.281	22.901	-21.602	5.967	-0.519
700	79.991	413.705	369.630	30.853	-21.456	10.550	-0.787
800	80.680	424.434	375.824	38.888	-21.372	15.115	-0.987
900	81.169	433.966	381.764	46.982	-21.345	19.674	-1.142
1000	81.527	442.538	387.420	55.118	-21.375	24.233	-1.266
1100	81.798	450.321	392.790	63.284	-21.461	28.797	-1.367
1200	82.006	457.448	397.885	71.475	-21.608	33.372	-1.453
1300	82.170	464.019	402.723	79.684	-21.824	37.962	-1.525
1400	82.301	470.113	407.322	87.908	-22.120	42.572	-1.588
1500	82.407	475.795	411.699	96.144	-22.510	47.206	-1.644
1600	82.495	481.116	415.873	104.389	-23.007	51.869	-1.693
1700	82.568	486.120	419.860	112.642	-23.624	56.567	-1.738
1800	82.629	490.841	423.673	120.902	-24.370	61.305	-1.779
1900	82.681	495.310	427.327	129.168	-25.251	66.088	-1.817
2000	82.726	499.552	430.833	137.438	-26.268	70.921	-1.852
2100	82.765	503.589	434.202	145.713	-27.418	75.808	-1.886
2200	82.798	507.440	437.445	153.991	-28.693	80.753	-1.917
2300	82.827	511.122	440.569	162.272	-30.080	85.759	-1.948
2400	82.853	514.647	443.582	170.556	-81.825	91.895	-2.000
2500	82.875	518.030	446.493	178.843	-83.470	99.167	-2.072
2600	82.896	521.281	449.307	187.131	-85.145	106.506	-2.140
2700	82.914	524.410	452.031	195.422	-86.835	113.909	-2.204
2800	82.930	527.425	454.670	203.714	-88.522	121.375	-2.264
2900	82.944	530.336	457.230	212.007	-90.190	128.901	-2.322
3000	82.957	533.148	459.714	220.303	-91.825	136.484	-2.376
3100	82.969	535.868	462.127	228.599	-93.414	144.121	-2.428
3200	82.980	538.503	464.472	236.896	-94.946	151.807	-2.478
3300	82.989	541.056	466.755	245.195	-96.412	159.541	-2.525
3400	82.998	543.534	468.977	253.494	-97.805	167.319	-2.571
3500	83.007	545.940	471.141	261.794	-99.119	175.136	-2.614
3600	83.014	548.278	473.252	270.095	-100.349	182.989	-2.655
3700	83.021	550.553	475.310	278.397	-101.492	190.876	-2.695
3800	83.027	552.767	477.320	286.700	-102.547	198.792	-2.733
3900	83.033	554.924	479.282	295.003	-103.512	206.735	-2.769
4000	83.039	557.026	481.199	303.306	-104.388	214.701	-2.804
4100	83.044	559.076	483.074	311.610	-105.174	222.688	-2.837
4200	83.048	561.078	484.907	319.915	-585.722	237.718	-2.956
4300	83.053	563.032	486.702	328.220	-585.246	257.318	-3.126
4400	83.057	564.941	488.458	336.526	-584.688	276.906	-3.287
4500	83.061	566.808	490.179	344.831	-584.049	296.481	-3.441
4600	83.064	568.633	491.864	353.138	-583.332	316.040	-3.589
4700	83.068	570.420	493.517	361.444	-582.540	335.583	-3.730
4800	83.071	572.169	495.137	369.751	-581.675	355.109	-3.864
4900	83.074	573.882	496.727	378.058	-580.741	374.616	-3.993
5000	83.077	575.560	498.287	386.366	-579.740	394.102	-4.117
5100	83.079	577.205	499.818	394.674	-578.675	413.569	-4.236
5200	83.082	578.818	501.322	402.982	-577.550	433.014	-4.350
5300	83 084	580.401	502.799	411.290	-576.366	452.436	-4.459
5400	83.086	581 954	504.251	419.599	-575.128	471.836	-4.564
5500	83.088	583.479	505.677	427.907	-573.837	491.213	-4.665
5600	83.090	584 976	507.080	436.216	-572.496	510.566	-4.762
5700	83.092	586.446	508.460	444.525	-571.108	529.894	-4.856
5800	83.094	587.892	509.817	452.835	-569.675	549.197	-4.946
5900	83.096	589.312	511.152	461 144	-568.200	568.475	-5.033
6000	83.097	590.709	512.466	469.454	-566.685	587.728	-5.117

PREVIOUS. December 1964 (1 atm) CURRENT December 1964 (1 bar)

Potassium Borate (KBO$_2$) CRYSTAL $M_r = 81.9071$ Potassium Borate (KBO$_2$) B$_1$K$_1$O$_2$(cr)

$S°(298.15\ K) = 79.98 \pm 0.12\ J\cdot K^{-1}\cdot mol^{-1}$
$T_{fus} = 1220 \pm 3\ K$

$\Delta_f H°(0\ K) = -990.1 \pm 8\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -995.0 \pm 8\ kJ\cdot mol^{-1}$
$\Delta_{fus} H° = 31.38 \pm 4.2\ kJ\cdot mol^{-1}$

Enthalpy of Formation

Shartsis and Capps[1] measured the enthalpies of solution in 2N nitric acid of various K_2O–B_2O glass and crystalline mixtures containing 1.1–41.0 mole % of K_2O. When these results are extrapolated to 50 mole %, we obtain $\Delta_{sol}H°$ (25°C) = -11.9 ± 2 kcal·mol^{-1} for $KBO_2(cr) + HNO_3(27.75\ H_2O,\ aq) + H_2O(l) \rightarrow KNO_3(27.75\ H_2O,\ aq) + H_3BO_3(27.75\ H_2O,\ aq)$ which leads to $\Delta_f H°(KBO_2,\ cr,\ 298.15\ K) = -237.8 \pm 2$ kcal·mol^{-1}, using the following auxiliary data. $\Delta_f H°(HNO_3\ 27.75\ H_2O,\ aq) = -256.37$ kcal·mol^{-1}.[4] The value, $\Delta_f H°(KBO_2,\ cr,\ 298.15\ K) = -237.8 \pm 2$ kcal·mol^{-1}, is adopted in the tabulation. Since the enthalpies of formation of $LiBO_2(cr)$ and $NaBO_2(cr)$ derived from the enthalpy of solution data are in good agreement with those values[5] adopted, their enthalpy of solution data should be reasonably reliable, although the calorimetric treatment was loose.

Heat Capacity and Entropy

Paukov *et al.*[6] have measured low temperature heat capacities from 12.11 to 312.22 K in an adiabatic calorimeter The adopted C_p are derived from their experimental heat capacites by a polynomial curve fitting technique. The derived entropy $S°(298.15\ K)$ is 19.116 ± 0.03 cal·K^{-1}·mol^{-1} based on $S°(12.11\ K) = 0.0353$ cal·K^{-1}·mol^{-1} Heat capacities above 310 K are estimated by comparison with those of $NaBO_2(cr)$[5] since both $NaBO_2$ and KBO_2 have same type of crystal structure.[7]

Thermal analysis data[8] have been interpreted in terms of a crystal transition at 785°C. Details of these studies are not available and it is not clear how reliable this interpretation is. We note, however, that the reported temperature (785°C) is essentially the same as the eutectic temperature of KBO_2 with $K_2B_4O_7$.[9, 10] We tentatively adopt a single C_p curve without a transition.

Fusion Data

Our analysis of several sets of binary phase data[8, 9, 11–14] yields the enthalpy of fusion, $\Delta_{fus}H° = 7.5 \pm 1$ kcal·mol^{-1}. The adopted melting point (947°C) is a weighted average of the observed data[8–15] which vary from 940 to 950°C.

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[3] The heat of formation of $KNO_3(aq)$ is calculated from JANAF $\Delta_f H°(KNO_3,\ \infty H_2O,\ aq,\ 298.15\ K) = -109.86$ kcal·mol^{-1} with the enthalpy of dilution ϕ_L given by V. B. Parker, U. S. Nat. Bur. Stand. NSRDS–NBS 2, 66 pp. (1965).
[4] This value, −256.37 kcal·mol^{-1}, is extrapolated from the enthalpies of formation of $H_3BO_3\cdot 60\ H_2O$ and H_3BO_3 100 H_2O listed in reference 2.
[5] JANAF Thermochemical Tables: $LiBO_2(cr)$ and $NaBO_2(cr)$, 6–30–71.
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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0	0.	INFINITE	−12.108	−990.083	−990.083	INFINITE
100	35.012	25.125	130.260	−10.513	−993.150	−974.741	509.152
200	54.095	55.873	85.716	−5.968	−994.444	−955.739	249.613
298.15	67.028	79.981	79.981	0.	−994.955	−936.616	164.091
300	67.237	80.397	79.983	0.124	−994.961	−936.254	163.016
400	76.651	101.079	82.739	7.336	−997.561	−916.196	119.643
500	83.973	118.997	88.238	15.379	−997.415	−895.863	93.590
600	89.830	134.842	94.710	24.079	−996.896	−875.596	76.227
700	94.558	149.054	101.476	33.305	−996.076	−855.441	63.834
800	98.491	161.945	108.241	42.963	−995.014	−835.420	54.547
900	101.755	173.739	114.873	52.980	−993.767	−815.544	47.333
1000	104.474	184.607	121.310	63.297	−992.387	−795.814	41.569
1100	106.525	194.666	127.527	73.853	−1069.889	−771.617	36.641
1200	107.864	204.001	133.516	84.582	−1067.376	−744.612	32.412
1220.0200	107.989	205.785	134.686	86.741	--- CRYSTAL <--> LIQUID ---		
1300	108.575	212.662	139.275	95.403	−1064.859	−717.817	28.842
1400	109.383	220.738	144.809	106.301	−1062.343	−691.216	25.790
1500	110.190	228.312	150.126	117.280	−1059.820	−664.795	23.150
1600	110.997	235.449	155.237	128.339	−1057.284	−638.542	20.846
1700	111.804	242.203	160.156	139.479	−1054.735	−612.449	18.818
1800	112.611	248.616	164.894	150.700	−1052.169	−586.506	17.020
1900	113.417	254.726	169.462	162.001	−1049.588	−560.706	15.415
2000	114.223	260.564	173.873	173.383	−1046.990	−535.043	13.974

PREVIOUS: CURRENT: June 1971

Potassium Borate (KBO$_2$) B$_1$K$_1$O$_2$(cr)

Potassium Borate (KBO_2) LIQUID $M_r = 81.9071$ Potassium Borate (KBO_2) $B_1K_1O_2(l)$

$S°(298.15\ K) = [88.455]\ J·K^{-1}·mol^{-1}$ $\Delta_fH°(298.15\ K) = [-980.730]\ kJ·mol^{-1}$

$T_{fus} = 1220 \pm 3\ K$ $\Delta_{fus}H° = 31.38 \pm 4.2\ kJ·mol^{-1}$

Enthalpy of Formation

$\Delta_fH°(KBO_2, l, 298.15\ K)$ is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(1220\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The constant heat capacity of the liquid is estimated to be 36 $J·K^{-1}·mol^{-1}$ based on that of $LiBO_2(l)$[1] which was derived from high temperature enthalpy measurements. A glass transition is assumed at 812 K below which the heat capacities are assumed to be the same as the crystal.

$S°(KBO_2, l, 298.15\ K)$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Vaporization Data

The boiling point is calculated as the temperature at which the fugacity is 1 atm for $KOB_2(l) \rightarrow KBO_2(g)$. The enthalpy of vaporization is the difference in $\Delta_fH°$ at the boiling point between liquid and gas.

Reference

[1] JANAF Thermochemical Table· $LiBO_2(l)$, 6-30-71.

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200							
298.15	67.028	88.455	88.455	0.	−980.730	−924.917	162.042
300	67.237	88.871	88.457	0.124	−980.735	−924.571	160.982
400	76.651	109.553	91.213	7.336	−983.335	−905.360	118.228
500	83.973	127.471	96.712	15.379	−983.190	−885.875	92.547
600	89.830	143.316	103.184	24.079	−982.670	−866.455	75.432
700	94.558	157.528	109.950	33.305	−981.850	−847.147	63.215
800	98.491	170.420	116.715	42.964	−980.788	−827.974	54.061
812.000	98.910	171.890	117.520	44.149	GLASS <--> LIQUID TRANSITION		
812.000	146.440	171.890	117.520	44.149			
900	146.440	186.958	123.585	57.035	−975.486	−809.159	46.962
1000	146 440	202.387	130.707	71.679	−969.779	−790.986	41.317
1100	146.440	216.344	137.868	86.323	−1043.193	−768.766	36.506
1200	146.440	229.086	144.946	100.967	−1036.765	−744.103	32.390
1220.000	146.440	231.506	145.346	103.896	--- CRYSTAL <--> LIQUID ---		
1300	146.440	240.807	151.876	115.611	−1030.425	−719.972	28.929
1400	146.440	251.660	158.620	130.255	−1024.163	−696.326	25.980
1500	146.440	261.763	165.163	144.899	−1017.974	−673.126	23.440
1600	146.440	271.214	171.499	159.543	−1011.854	−650.336	21.231
1700	146.440	280.092	177.629	174.187	−1005.801	−627.927	19.294
1800	146.440	288.462	183.556	188.831	−999.812	−605.872	17.582
1900	146.440	296.380	189.287	203.475	−993.888	−584.148	16.059
2000	146 440	303.891	194.832	218.119	−988.029	−562.735	14.697

PREVIOUS: CURRENT June 1971

Potassium Borate (KBO$_2$) **CRYSTAL-LIQUID**

0 to 1220 K crystal
above 220 K liquid

Refer to the individual tables for details.

$M_r = 81.9071$ Potassium Borate (KBO$_2$) **$B_1K_1O_2(cr,l)$**

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−12.98	−990.083	−990.083	INFINITE
100	35.012	25.125	130.260	−10.513	−993.150	−974.741	509.152
200	54.095	55.873	85.716	−5.968	−994.444	−955.739	249.613
298.15	67.028	79.981	79.981	0.	−994.955	−936.616	164.091
300	67.237	80.397	79.983	0.124	−994.961	−936.254	163.016
400	76.651	101.079	82.739	7.336	−997.561	−916.196	119.643
500	83.973	118.997	88.238	15.379	−997.415	−895.863	93.590
600	89.830	134.842	94.710	24.079	−996.896	−875.596	76.227
700	94.558	149.054	101.476	33.305	−996.076	−855.441	63.834
800	98.491	161.945	108.241	42.963	−995.014	−835.420	54.547
900	101.755	173.739	114.873	52.980	−993.767	−815.544	47.333
1000	104.474	184.607	121.310	63.297	−992.387	−795.814	41.569
1100	106.525	194.666	127.527	73.853	−1069.889	−771.617	36.641
1200	107.864	204.001	133.516	84.582	−1067.376	−744.612	32.412
1220.000	107.989	205.785	134.686	86.741	____ CRYSTAL <--> LIQUID ____		
1220.000	146.440	231.506	134.686	118.121		TRANSITION	
1300	146.440	240.807	140.933	129.836	−1030.426	−719.973	28.929
1400	146.440	251.660	148.460	144.480	−1024.164	−696.327	25.980
1500	146.440	261.763	155.680	159.124	−1017.975	−673.127	23.440
1600	146.440	271.214	162.609	173.768	−1011.855	−650.337	21.231
1700	146.440	280.092	169.261	188.412	−1005.802	−627.928	19.294
1800	146.440	288.462	175.653	203.056	−999.813	−605.873	17.582
1900	146.440	296.380	181.801	217.700	−993.889	−584.149	16.059
2000	146.440	303.891	187.719	232.344	−988.030	−562.736	14.697

PREVIOUS: CURRENT: June 1971

Potassium Borate (KBO$_2$) **$B_1K_1O_2(cr,l)$**

Potassium Borate (KBO_2) IDEAL GAS $M_r = 81.9071$ Potassium Borate (KBO_2) $B_1K_1O_2(g)$

$S°(298.15\ K) = [297.4 \pm 4]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -671 \pm 25\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -674 \pm 25\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	 ν, cm^{-1}
1952(1)	577(1)
1081(1)	265(1)
581(1)	88(1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: C_s
Bond Distances: K–O = [2.4] Å; O–B = [1.36] Å; B–O = [1.20] Å
Bond Angles: K–O–B = [90]°; O–B–O = [180]°
Product of the Moments of Inertia: $I_A I_B I_C = [5.790543 \times 10^{-114}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

Jensen[1] determined the equilibrium constants for the reaction: $K(g) + HBO_2(g) \rightarrow KBO_2(g) + H(g)$ by flame studies. This technique involved several assumptions, the most basic of which is that boron added to $H_2/N_2/O_2$ flames was converted completely to HBO_2. The hydrogen atom concentration was taken from previous studies on such flames. Potassium metaborate was assumed to be formed in the flame. The concentration of K atom was determined by atomic absorption spectrophotometry. JANAF 3rd law analysis of his equilibrium constant equation in the temperature range from 2000 to 2600 K yields $\Delta_r H°(298.15\ K) = 3.66 \pm 0.54\ kcal{\cdot}mol^{-1}$and the drift is $1.26\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. (2nd law enthalpy of reaction is $\Delta_r H°(298.15\ K) = 0.78\ kcal{\cdot}mol^{-1}$.) Using the 3rd law $\Delta_r H°(298.15\ K)$ and JANAF auxiliary data, we obtain $\Delta_f H°(KBO_2,\ g,\ 298.15\ K) = -161.1\ kcal{\cdot}mol^{-1}$. The uncertainty in this measurement was about $\pm 6\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

Seshadri, Nimon and White[2] observed the infrared spectra of KBO_2 in an argon matrix and made a complete assignment of all six fundamentals which are adopted in the tabulation. The uncertainty of the calculated statistical entropy at 298.15 K is estimated to be ±1 eu which is due to the magnitude of the matrix shifts from the free molecule spectrum, particularly for the lower frequency modes.

The molecular structure, bond distance and bond angle of $KBO_2(g)$ are assumed to be the same as those of $LiBO_2(g)$ and $NaBO_2(g)$,[1] except the bond distance K–O which was estimated to be intermediate between those of potassium fluoride and chloride. The principal moments of inertia are: $I_A = 6.1073 \times 10^{-39}$, $I_B = 27.8891 \times 10^{-39}$, and $I_C = 33.9965 \times 10^{-39}\ g{\cdot}cm^2$

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[3] JANAF Thermochemical Tables: $LiBO_2(g)$ and $NaBO_2(g)$, 6–30–71.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−14.103	−671.166	−671.166	INFINITE
100	43.615	242.225	345.119	−10.289	−672.013	−675.314	352.748
200	52.329	275.193	302.607	−5.483	−673.045	−678.205	177.129
250	56.018	287.277	298.364	−2.772	−673.537	−679.438	141.961
298.15	59.027	297.408	297.408	0.	−674.042	−680.529	119.226
300	59.133	297.774	297.410	0.109	−674.063	−680.569	118.498
350	61.757	307.092	298.139	3.133	−677.034	−681.511	101.710
400	63.992	315.488	299.792	6.279	−677.706	−682.105	89.074
450	65.921	323.139	301.967	9.528	−678.366	−682.615	79.236
500	67.602	330.174	304.441	12.867	−679.015	−683.052	71.358
600	70.385	342.756	309.803	19.772	−680.291	−683.739	59.525
700	72.568	353.776	315.314	26.924	−681.544	−684.215	51.057
800	74.296	363.584	320.746	34.270	−682.794	−684.511	44.694
900	75.672	372.417	326.004	41.771	−684.063	−684.650	39.736
1000	76.776	380.449	331.053	49.395	−685.376	−684.645	35.762
1100	77.669	387.810	335.883	57.119	−765.710	−679.895	32.286
1200	78.397	394.600	340.497	64.924	−766.122	−672.076	29.255
1300	78.997	400.900	344.904	72.794	−766.554	−664.222	26.689
1400	79.495	406.773	349.116	80.720	−767.011	−656.333	24.488
1500	79.911	412.272	353.145	88.691	−767.496	−648.411	22.580
1600	80.263	417.441	357.003	96.700	−768.011	−640.455	20.909
1700	80.562	422.316	360.703	104.741	−768.559	−632.466	19.433
1800	80.818	426.928	364.256	112.811	−769.146	−624.444	18.121
1900	81.038	431.304	367.670	120.904	−769.773	−616.388	16.946
2000	81.230	435.466	370.957	129.017	−770.443	−608.298	15.887
2100	81.397	439.433	374.124	137.149	−771.161	−600.174	14.929
2200	81.543	443.223	377.179	145.296	−771.930	−592.013	14.056
2300	81.672	446.851	380.130	153.457	−772.752	−583.817	13.259
2400	81.787	450.329	382.983	161.630	−823.891	−574.516	12.504
2500	81.888	453.670	385.744	169.814	−824.908	−564.104	11.786
2600	81.979	456.883	388.419	178.007	−825.956	−553.651	11.123
2700	82.061	459.979	391.012	186.209	−827.039	−543.157	10.508
2800	82.134	462.964	393.529	194.419	−828.159	−532.622	9.936
2900	82.200	465.848	395.973	202.636	−829.320	−522.048	9.403
3000	82.260	468.636	398.349	210.859	−830.526	−511.432	8.905
3100	82.314	471.334	400.660	219.088	−831.780	−500.774	8.438
3200	82.364	473.948	402.910	227.322	−833.085	−490.076	8.000
3300	82.409	476.483	405.101	235.560	−834.436	−479.338	7.587
3400	82.451	478.944	407.237	243.803	−835.852	−468.555	7.198
3500	82.489	481.334	409.320	252.051	−837.326	−457.732	6.831
3600	82.524	483.659	411.353	260.301	−838.868	−446.864	6.484
3700	82.557	485.920	413.338	268.555	−840.479	−435.954	6.155
3800	82.586	488.122	415.277	276.812	−842.165	−424.997	5.842
3900	82.614	490.268	417.172	285.072	−843.928	−413.996	5.545
4000	82.640	492.360	419.026	293.335	−845.768	−402.950	5.262
4100	82.664	494.401	420.840	301.600	−847.696	−391.856	4.992
4200	82.686	496.393	422.615	309.868	−1329.568	−373.690	4.648
4300	82.707	498.339	424.353	318.138	−1330.600	−350.919	4.263
4400	82.726	500.240	426.057	326.409	−1331.457	−328.150	3.896
4500	82.744	502.100	427.726	334.683	−1332.630	−305.335	3.544
4600	82.761	503.919	429.363	342.958	−1333.904	−282.493	3.208
4700	82.777	505.699	430.968	351.235	−1335.260	−259.623	2.885
4800	82.792	507.442	432.543	359.513	−1336.612	−236.736	2.576
4900	82.806	509.149	434.089	367.793	−1338.175	−213.805	2.279
5000	82.819	510.822	435.607	376.075	−1339.846	−190.842	1.994
5100	82.832	512.462	437.098	384.357	−1341.626	−167.844	1.719
5200	82.844	514.071	438.563	392.641	−1343.518	−144.811	1.455
5300	82.855	515.649	440.002	400.926	−1345.523	−121.739	1.200
5400	82.865	517.198	441.418	409.212	−1347.643	−98.630	0.954
5500	82.875	518.718	442.809	417.499	−1349.876	−75.480	0.717
5600	82.885	520.211	444.178	425.787	−1352.225	−52.287	0.488
5700	82.894	521.679	445.525	434.076	−1354.344	−29.101	0.267
5800	82.902	523.120	446.850	442.365	−1356.878	−5.828	0.052
5900	82.910	524.538	448.155	450.656	−1359.522	17.487	−0.155
6000	82.918	525.931	449.440	458.947	−1362.276	40.850	−0.356

PREVIOUS June 1971 (1 atm) CURRENT June 1971 (1 bar)

Potassium Borate (KBO_2) $B_1K_1O_2(g)$

Lithium Borate ($LiBO_2$) CRYSTAL $M_r = 49.7498$

$S°(298.15\ K) = 51.73 \pm 0.2\ J\cdot K^{-1}\cdot mol^{-1}$
$T_{fus} = 1117 \pm 1\ K$

$\Delta_f H°(0\ K) = -1013.7 \pm 0.8\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -1019.2 \pm 0.8\ kJ\cdot mol^{-1}$
$\Delta_{fus} H° = 33.81 \pm 0.5\ kJ\cdot mol^{-1}$

Enthalpy of Formation

Sinke[1] measured calorimetrically the enthalpy of solution of $LiBO_2(cr)$ in 0.5 N HNO_3, $\Delta_{sol}H°(25°C) = -10\ 93 \pm 0.05\ kcal\cdot mol^{-1}$ for $LiBO_2(cr) + HNO_3(aq,\ 111\ H_2O) \rightarrow H_3BO_3(aq,\ 111\ H_2O) + LiNO_3(aq,\ 111\ H_2O)$, which leads to the adopted enthalpy of formation, $\Delta_f H°(LiBO_2,\ cr,\ 298.15\ K) = -243.6 \pm 0.2\ kcal\cdot mol^{-1}$ using the following auxiliary data: $\Delta_f H°(HNO_3\cdot 111\ H_2O,\ aq,\ 298.15\ K) = -49.411\ kcal\cdot mol^{-1}$,[2] $\Delta_f H°(H_2O,\ l,\ 298.15\ K) = -68.315\ kcal\cdot mol^{-1}$,[2] $\Delta_f H°(H_3BO_3\cdot 111\ H_2O,\ aq,\ 298.15\ K) = -256.336\ kcal\cdot mol^{-1}$ [2] and $\Delta_f H°(LiNO_3\cdot 111\ H_2O,\ aq,\ 298.15\ K) = -115.944\ kcal\cdot mol^{-1}$.[3]

Shartsis and Capps[4] measured enthalpies of solution in 2N nitric acid of various Li_2O–B_2O_3 glass and crystalline mixtures containing 2.5–48.4 mole % of Li_2O. When their results are extrapolated to 50 mole %, we obtain $\Delta_{sol}H°(25°C) = -10.8 \pm 0.5\ kcal\ mol^{-1}$ for $LiBO_2(cr) + HNO_3(27.75\ H_2O,\ aq) + H_2O(l) \rightarrow LiNO_3(27.75\ H_2O,\ aq) + H_3BO_3(27.75\ H_2O,\ aq)$ The calculated enthalpy of formation is based on the following data: $\Delta_f H°(HNO_3\cdot 27.75\ H_2O,\ aq,\ 298.15\ K) = -49.433\ kcal\cdot mol^{-1}$,[2] $\Delta_f H°(LiNO_3\cdot 27.75\ H_2O,\ aq,\ 298.15\ K) = -115.854\ kcal\cdot mol^{-1}$ [5] and $\Delta_f H°(H_3BO_3\cdot 27.75\ H_2O,\ aq,\ 298.15\ K) = -256.37\ kcal\cdot mol^{-1}$.[6] The value is $\Delta_f H°(LiBO_2,\ cr,\ 298.15\ K) = -243.9 \pm 0.5\ kcal\cdot mol^{-1}$, which is in very good agreement with the adopted value.

Heat Capacity and Entropy

Stull *et al.*[7] measured low temperature C_p data from 15 to 320 K. We use their smoothed C_p values to derive $S°(298.15\ K) = 12.36 \pm 0.05\ cal\cdot K^{-1}\cdot mol^{-1}$ based on $S°(15\ K) = 0.017\ cal\ K^{-1}\cdot mol^{-1}$. McDonald[8] determined high temperature enthalpy data from 288 to 1116 K by drop calorimetry. The low temperature C_p and high temperature enthalpy data are smoothly joined at 298.15 K by a polynomial curve fitting technique. The average deviation of the observed enthalpy data from the adopted values is about 0.3% in the temperature range from 428–1062 K, and the maximum is 0.56% at 922 K. The C_p values above T_{fus} are extrapolated from the adopted polynomial function.

Turdakin and Tarasov[9] also measured low temperature heat capacities (55–300 K) in an adiabatic calorimeter. Their values deviate from the adopted C_p by approximately 2%.

Melting curves from binary phase studies[10–12] have been interpreted in terms of a crystal transition near 800°C, although the most recent paper[13] indicated no transition. Two high-pressure polymorphs have been observed[14] but there is no evidence of their stability at atmospheric pressure. Enthalpy data[8] showed no obvious transition near 800°C; points at 829 and 815°C showed reasonable premelting contributions of about 200 and 300 $kcal\cdot mol^{-1}$, respectively. Although this evidence does not preclude the existence of a transition, definite evidence would be needed to establish such a transition.

Fusion Data

Refer to the liquid table for details.

References

[1] G. C. Sinke, Thermal Research Lab., The Dow Chemical Company, Midland, Michigan, personal communication, (April, 1961).
[2] U. S. Nat. Bur. Stand. Tech. Note 270–3, 264 pp. (1968).
[3] This value, ($LiNO_3\cdot 111\ H_2O$, aq $\Delta_f H°298.15\ K) = -115.944\ kcal\cdot mol^{-1}$, is calculated based on the follwoing auxiliary data:
  a. $\phi_L = 0.171\ kcal\ mol^{-1}$ for $LiNO_3(\infty\ H_2O) \rightarrow LiNO_3\cdot(111\ H_2O)$ ϕ_L was obtained fromV.B. Parker, U. S. Nat. Bur. Stand., NSRDS–NBS 2, 66 pp. (1965).
  b. $\Delta_f H°(LiNO_3\ [aq,\ \infty],\ 298.15\ K) = -116.115\ kcal\cdot mol^{-1}$.
    This value is the sum of $\Delta_f H°(Li+\ [aq,\ \infty]\ 298.15\ K) = -66.555\ kcal\cdot mol^{-1}$ and $\Delta_f H°(NO_3^-\ [aq,\ \infty],\ 298.15\ K) = 49.56\ kcal\cdot mol^{-1}$.[2]
    The former is derived from $\Delta_f H°(LiOH\ [aq,\ \infty],\ 298.15\ K = -121.525\ kcal\cdot mol^{-1}$ and $\Delta_f H°(OH^-\ [aq,\ \infty] = -54.97\ kcal\cdot mol^{-1}$.[2]
[4] L. Shartsis and W. Capps J. Am. Chem. Soc. 37, 27 (1954).
[5] This value, $-115.854\ kcal\cdot mol^{-1}$, is calculated from $\Delta_f H°(LiNO_3\ [aq,\ \infty],\ 298.15\ K = -116.115\ kcal\cdot mol^{-1}$ and $\phi_L = 0.261\ kcal\cdot mol^{-1}$ for $LiNO_3(\infty\ H_2O) \rightarrow LiNO_3\cdot(27\ 75\ H_2O)$ reported by V. B. Parker, U. S. Nat. Bur. Stand. NSRDS–NBS 2, 66 pp. (1965).
[6] This value, $-256.37\ kcal\cdot mol^{-1}$, is extrapolated from the enthalpies of formation of $H_3BO_3\cdot 60H_2O$ and $H_3BO_3\cdot 100\ H_2O$ listed by NBS.[2]
[7] D. R. Stull, D. L. Hildenbrand, F. L. Oetting and G. C. Sinke, J. Chem. Eng. Data 15, 52 (1970).
[8] R. A. McDonald, Thermal Res. Laboratory, The Dow Chemical Company, personal communication, April, 1961, CPIA Publication No. 44(U), Vol. 1, pp. 213–245, (February, 1964).
[9] V. A. Turdakin and V. V. Tarasov, Russ. J. Phys. Chem. 42, 1483 (1968).
[10] I. I. Kitaigorodskii, T. A. Popova and O. K. Botvinkin, J. Phys. Chem., USSR 4, 380 (1933).
[11] A. G. Bergman, A. I. Kislova and V. I. Posypaiko, Russ. J. Gen. Chem. 25, 1831, 1993 (1955).
[12] A. G. Bergman and D. I. Bondareva, Russ. J. Inorg. Chem. 14, 586, 1339 (1969).
[13] A. G. Bergman and D. I. Bondareva, Russ. J. Inorg. Chem. 15, 1339 (1970).
[14] C. H. Chang and J. L. Margrave, J. Amer. Chem. Soc. 90, 2020 (1968).

Lithium Borate ($LiBO_2$) $B_1Li_1O_2(cr)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J\cdot K^{-1}mol^{-1}$			$kJ\cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0	0.	0.	INFINITE	−8.975	−1013.678	−1013.678	INFINITE
100	18.795	10.192	93.035	−8.284	−1016.411	−999.334	521.999
200	43.133	31.104	56.731	−5.125	−1018.338	−981.412	256.319
298.15	60.371	51.731	51.731	0.	−1019.222	−963.070	168.726
300	60.618	52.105	51.732	0.112	−1019.231	−962.722	167.625
400	71.145	71.112	54.252	6.744	−1019.534	−943.833	123.252
500	78.605	87.818	59.329	14.244	−1022.756	−924.575	96.590
600	85.057	102.728	65.341	22.432	−1022.692	−904.938	78.782
700	91.098	116.297	71.665	31.242	−1022.217	−885.344	66.065
800	96.939	128.844	78.038	40.645	−1021.330	−865.847	56.534
900	102.675	140.594	84.342	50.627	−1020.027	−846.485	49.129
1000	108.353	151.706	90.528	61.178	−1018.286	−827.292	43.213
1100	113.989	162.298	96.574	72.296	−1016.088	−808.295	38.383
1117.000	114.943	164.053	97.588	74.241	--- CRYSTAL <--> LIQUID ---		
1200	119.604	172.457	102.477	83.975	−1013.422	−789.519	34.367
1300	125.202	182.251	108.239	96.216	−1010.279	−770.984	30.979
1400	130.788	191.734	113.866	109.015	−1006.649	−752.710	28.084
1500	136.369	200 948	119.366	122.373	−1002.524	−734.713	25.585
1600	141 938	209.927	124.747	136.288	−997.901	−717.007	23.408
1700	147.507	218.699	130.016	150.761	−1138.015	−692.429	21.276
1800	153.072	227.288	135.182	165.790	−1131.636	−666.400	19.338
1900	158.636	235.713	140.252	181.375	−1124.764	−640.739	17.615
2000	164.193	243.991	145.233	197.517	−1117.396	−615.452	16.074

PREVIOUS: December 1964 CURRENT June 1971

Lithium Borate ($LiBO_2$) LIQUID $M_r = 49.7498$ Lithium Borate ($LiBO_2$) $B_1Li_1O_2(l)$

$S°(298.15\ K) = [65.547]\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{fus} = 1117 \pm 1\ K$

$\Delta_f H°(298.15\ K) = [-1000.259]\ kJ \cdot mol^{-1}$
$\Delta_{fus} H° = 33.81 \pm 0.5\ kJ \cdot mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(LiBO_2, l, 298.15\ K)$ is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(1117\ K)–H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

McDonald[1] measured high temperature enthalpy data of the liquid from 1118 to 1707 K by drop calorimetry. The adopted heat capacities are derived from his observed data. The average deviation of the observed enthalpy data from the adopted values is about 0.1%. A glass transition is assumed at 745 K below which the C_p is assumed to be the same as that of the crystal.

$S°(LiBO_2, l, 298.15\ K)$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

The adopted enthalpy of fusion, $\Delta_{fus}H°(1117\ K) = 8.08 \pm 0.12\ kcal \cdot mol^{-1}$, is calculated from the observed enthalpies[1] by use of the adopted C_p functions of both crystal and liquid.

Petit and Jaeger[2] derived $\Delta_{fus}H°(1109\ K) = 7.4\ kcal \cdot mol^{-1}$ from phase data for the $LiBO_2$–LiF system. Darmois and Zarzycki[3] determined $\Delta_{fus}H°(1113\ K) = 8.3 \pm 0.6\ kcal \cdot mol^{-1}$ from cryoscopic studies involving several secondary components.

Vaporization Data

The boiling point is calculated as the temperature at which the fugacity is 1 atm for $LiBO_2(l) \rightarrow LiBO_2(g)$. The enthalpy of vaporization is the difference in $\Delta_f H°$ at the boiling point between liquid and gas.

Prophet[4] determined the boiling point under argon atmosphere as 2050 ± 100 K which is in good agreement with the value calculated.

References

[1] R. A. McDonald, Thermal Res. Laboratory, The Dow Chemical Company, personal communication, April, 1961; CPTA Publication No. 44(U), Vol. 1, pp. 213–245, (1964).

[2] C. Petit and M. Jaeger, Compt. Rend. 244, 1734 (1957).

[3] G. Zarzycki, Compt. Rend. 233, 1110 (1951).

[4] H. Prophet, Thermal Res. Laboratory, The Dow Chemical Company,personal communication, (April, 1961).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	60.371	65.547	65.547	0.	−1000.259	−948.226	166.125
300	60.618	65.921	65.548	0.112	−1000.268	−947.903	165.045
400	71.145	84.928	68.069	6.744	−1000.570	−930.396	121.497
500	78.605	101.634	73.146	14.244	−1003.793	−912.520	95.330
600	85.057	116.544	79.158	22.432	−1003.729	−894.264	77.853
700	91.098	130.113	85.482	31.242	−1003.254	−876.052	65.372
745.000	93.741	135.871	88.352	35.401	GLASS <--> LIQUID TRANSITION		
745.000	144.310	135.871	88.352	35.401			
800	144.310	146.149	91.977	43.338	−999.673	−858.034	56.024
900	144.310	163.147	98.959	57.769	−993.921	−840.677	48.792
1000	144.310	178.351	106.151	72.200	−988.300	−823.952	43.039
1100	144.310	192.106	113.350	86.631	−982.789	−807.784	38.358
1117.000	144.310	194.319	114.565	89.085	--- CRYSTAL <--> LIQUID ---		
1200	144.310	204.662	120.444	101.062	−977.372	−792.115	34.480
1300	144.310	216.213	127.372	115.493	−972.038	−776.894	31.216
1400	144.310	226.908	134.105	129.924	−966.776	−762.080	28.434
1500	144.310	236.864	140 627	144.355	−961.578	−747.641	26.035
1600	144.310	246.178	146.936	158.786	−956.440	−733.546	23.948
1700	144.310	254.927	153.034	173.218	−1096.594	−712.595	21.895
1800	144.310	263.175	158.926	187.649	−1090.814	−690.175	20.028
1900	144.310	270.978	164.620	202.080	−1085.096	−668.073	18.367
2000	144.310	278.380	170.124	216.511	−1079.438	−646.271	16.879
2100	144.310	285.421	175.448	230.942	−1073.842	−624.751	15.540
2200	144.310	292.134	180.601	245.373	−1068.306	−603.495	14.329
2300	144.310	298.549	185.591	259.804	−1062.832	−582.490	13.229
2400	144.310	304.691	190.426	274.235	−1107.678	−560.653	12.202
2500	144.310	310.582	195.115	288.666	−1102.406	−537.969	11.240
2600	144.310	316.242	199.666	303.097	−1097.164	−515.495	10.356
2700	144.310	321.688	204.085	317.528	−1091.954	−493.222	9.542
2800	144.310	326.936	208.379	331.959	−1086.777	−471.141	8.789
2900	144.310	332.000	212.555	346.390	−1081.634	−449.246	8.092
3000	144.310	336.893	216.619	360.821	−1076.526	−427.526	7.444

PREVIOUS December 1964 CURRENT: June 1971

Lithium Borate ($LiBO_2$) $B_1Li_1O_2(l)$

Lithium Borate ($LiBO_2$) CRYSTAL-LIQUID

0 to 1117 K crystal
above 1117 K liquid

Refer to the individual tables for details.

$M_r = 49.7498$ Lithium Borate ($LiBO_2$) $B_1Li_1O_2(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−8.975	−1013.678	−1013.678	INFINITE
100	18.795	10.192	93.035	−8.284	−1016.411	−999.334	521.999
200	43.133	31.104	56.731	−5.125	−1018.338	−981.412	256.319
298.15	60.371	51.731	51.731	0.	−1019.222	−963.070	168.726
300	60.618	52.105	51.732	0.112	−1019.231	−962.722	167.625
400	71.145	71.112	54.252	6.744	−1019.534	−943.833	123.252
500	78.605	87.818	59.329	14.244	−1022.756	−924.575	96.590
600	85.057	102.728	65.341	22.432	−1022.692	−904.938	78.782
700	91.098	116.297	71.665	31.242	−1022.217	−885.344	66.065
800	96 939	128.844	78.038	40.645	−1021.330	−865.847	56.534
900	102.675	140.594	84.342	50.627	−1020.027	−846.485	49.129
1000	108.353	151.706	90.528	61.178	−1018.286	−827.292	43.213
1100	113.989	162.298	96.574	72.296	−1016.088	−808.295	38.383
1117.000	114.943	164.053	97.588	74.241	CRYSTAL <−−> LIQUID TRANSITION		
1117.000	144.310	194.319	97.588	108.048			
1200	144.310	204.662	104.641	120.026	−977.372	−792.115	34.480
1300	144.310	216.213	112.785	134.457	−972.038	−776.894	31.216
1400	144.310	226.908	120.559	148.888	−966.776	−762.080	28.434
1500	144.310	236.864	127.985	163.319	−961.578	−747.641	26.035
1600	144.310	246.178	135.084	177.750	−956.440	−733.546	23.948
1700	144.310	254.927	141.879	192.181	−1096.594	−712.595	21.895
1800	144.310	263.175	148.391	206.612	−1090.814	−690.175	20.028
1900	144.310	270.978	154.639	221.043	−1085.096	−668.073	18.367
2000	144.310	278.380	160.643	235.474	−1079.438	−646.271	16.879
2100	144.310	285.421	166.418	249.905	−1073.842	−624.751	15.540
2200	144.310	292.134	171.981	264.336	−1068.306	−603.495	14.329
2300	144.310	298.549	177.346	278.767	−1062.832	−582.490	13.229
2400	144.310	304.691	182.525	293.198	−1107.678	−560.653	12.202
2500	144.310	310.582	187.530	307.629	−1102.406	−537.969	11.240
2600	144.310	316.242	192.372	322.060	−1097.164	−515.495	10.356
2700	144.310	321.688	197.061	336.491	−1091.954	−493.222	9.542
2800	144.310	326.936	201.607	350.923	−1086.777	−471.141	8.789
2900	144.310	332.000	206.016	365.354	−1081.634	−449.246	8.092
3000	144.310	336.893	210.298	379.785	−1076.526	−427.526	7.444

PREVIOUS: CURRENT: June 1971

Lithium Borate ($LiBO_2$) $B_1Li_1O_2(cr,l)$

Lithium Borate (LiBO$_2$) IDEAL GAS $M_r = 49.7498$ Lithium Borate (LiBO$_2$) B$_1$Li$_1$O$_2$(g)

$\Delta_f H°(0\ \text{K}) = -645.8 \pm 12.6\ \text{kJ·mol}^{-1}$
$S°(298.15\ \text{K}) = 274.7 \pm 42\ \text{J·K}^{-1}\text{·mol}^{-1}$ $\Delta_f H°(298.15\ \text{K}) = -646.8 \pm 12.6\ \text{kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}
1976(1)	569(1)
1094(1)	471(1)
578(1)	107(1)

Ground State Quantum Weight: 1 $\sigma = 1$
Point Group: C_s
Bond Distances: Li-O = 1.82 Å; O-B = 1.36 Å; B-O = 1.20 Å
Bond Angles: Li-O-B = 90°; O-B-O = 180°
Product of the Moments of Inertia: $I_A I_B I_C = 3.915323 \times 10^{-115}\ \text{g}^3\text{·cm}^6$

Enthalpy Reference Temperature = T_r = 298.15 K				Standard State Pressure = $p°$ = 0.1 MPa			
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−13.445	−645.772	−645.772	INFINITE
100	40.840	222.599	320.197	−9.760	−645.510	−649.674	339.355
200	49.547	253.423	279.734	−5.262	−646.098	−653.637	170.712
250	53.797	264.948	275.651	−2.676	−646.469	−655.479	136.955
298.15	57.246	274.727	274.727	0.	−646.846	−657.181	115.135
300	57.366	275.082	274.728	0.106	−646.861	−657.245	114.436
350	60.331	284.154	275.438	3.051	−647.283	−658.943	98.342
400	62.816	292.377	277.050	6.131	−647.770	−660.576	86.262
450	64.932	299.901	279.176	9.326	−648.343	−662.143	76.860
500	66.756	306.839	281.600	12.619	−652.005	−663.335	69.298
600	69.739	319.286	286.868	19.451	−653.298	−665.478	57.935
700	72.055	330.217	292.296	26.545	−654.538	−667.410	49.803
800	73.876	339.963	297.656	33.845	−655.754	−669.166	43.692
900	75.323	348.751	302.853	41.308	−656.970	−670.769	38.930
1000	76.481	356.749	307.849	48.900	−658.188	−672.237	35.114
1100	77.416	364.084	312.632	56.597	−659.411	−673.582	31.986
1200	78.179	370.853	317.205	64.378	−660.644	−674.816	29.374
1300	78.806	377.137	321.577	72.228	−661.891	−675.947	27.160
1400	79.327	382.996	325.757	80.135	−663.153	−676.981	25.258
1500	79.762	388.485	329.758	88.090	−664.431	−677.925	23.607
1600	80.130	393.645	333.591	96.085	−665.728	−678.782	22.160
1700	80.443	398.512	337.268	104.115	−812.285	−672.381	20.660
1800	80.711	403.118	340.800	112.173	−812.878	−664.135	19.273
1900	80.941	407.488	344.196	120.255	−813.507	−655.855	18.031
2000	81.142	411.645	347.465	128.360	−814.177	−647.540	16.912
2100	81.316	415.608	350.616	136.483	−814.888	−639.191	15.899
2200	81.469	419.395	353.657	144.622	−815.644	−630.806	14.977
2300	81.604	423.019	356.595	152.776	−816.447	−622.387	14.135
2400	81.724	426.495	359.435	160.943	−867.558	−612.863	13.339
2500	81.830	429.833	362.185	169.121	−868.539	−602.231	12.583
2600	81.925	433.044	364.849	177.308	−869.540	−591.559	11.885
2700	82.011	436.138	367.432	185.505	−870.564	−580.847	11.237
2800	82.087	439.122	369.940	193.710	−871.613	−570.098	10.635
2900	82.156	442.004	372.375	201.922	−872.689	−559.311	10.074
3000	82.219	444.790	374.743	210.141	−873.793	−548.486	9.550
3100	82.276	447.487	377.046	218.366	−874.927	−537.623	9.059
3200	82.328	450.100	379.288	226.596	−876.093	−526.724	8.598
3300	82.375	452.634	381.473	234.832	−877.292	−515.789	8.164
3400	82.419	455.094	383.602	243.071	−878.526	−504.815	7.756
3500	82.459	457.483	385.679	251.315	−879.795	−493.805	7.370
3600	82.496	459.807	387.706	259.563	−881.101	−482.759	7.005
3700	82.529	462.068	389.685	267.814	−882.446	−471.676	6.659
3800	82.561	464.269	391.619	276.069	−883.830	−460.554	6.331
3900	82.590	466.414	393.510	284.326	−885.254	−449.397	6.019
4000	82.617	468.505	395.359	292.587	−886.720	−438.203	5.722
4100	82.642	470.546	397.168	300.850	−888.230	−426.971	5.440
4200	82.665	472.537	398.939	309.115	−1369.633	−408.678	5.083
4300	82.686	474.483	400.673	317.382	−1370.146	−385.792	4.686
4400	82.707	476.384	402.372	325.652	−1370.688	−362.896	4.308
4500	82.726	478.243	404.037	333.924	−1371.291	−339.985	3.946
4600	82.743	480.061	405.670	342.197	−1371.948	−317.061	3.600
4700	82.760	481.841	407.272	350.472	−1372.659	−294.120	3.269
4800	82.776	483.583	408.844	358.749	−1373.425	−271.165	2.951
4900	82.790	485.290	410.387	367.028	−1374.248	−248.192	2.646
5000	82.804	486.963	411.902	375.307	−1375.132	−225.202	2.353
5100	82.817	488.603	413.390	383.588	−1376.072	−202.195	2.071
5200	82.830	490.211	414.851	391.871	−1377.080	−179.169	1.800
5300	82.841	491.789	416.288	400.154	−1378.156	−156.121	1.539
5400	82.852	493.338	417.701	408.439	−1379.302	−133.054	1.287
5500	82.863	494.858	419.090	416.725	−1380.521	−109.964	1.044
5600	82.873	496.351	420.456	425.011	−1381.815	−86.851	0.810
5700	82.882	497.818	421.801	433.299	−1383.187	−63.715	0.584
5800	82.891	499.260	423.124	441.588	−1384.640	−40.553	0.365
5900	82.899	500.677	424.426	449.877	−1386.177	−17.368	0.154
6000	82.907	502.070	425.709	458.168	−1387.802	5.847	−0.051

PREVIOUS: June 1971 (1 atm) CURRENT: June 1971 (1 bar)

Enthalpy of Formation

Jensen[1] determined the equilibrium constants for reaction (A) Li(g) + HBO$_2$(g) LiBO$_2$(g) + H(g) by flame studies. This technique involves several assumptions, the most basic of which is that boron added to H$_2$/N$_2$/O$_2$ flames is converted completely to HBO$_2$. The hydrogen atom concentration was taken from previous studies on such flames. Lithium metaborate was assumed to be formed in the flame. The concentration of Li atoms was determined by atomic absorption spectrophotometry. JANAF 3rd law analysis of his equilibrium constant equation in the temperature range from 2000 to 2600 K yields $\Delta_r H°(298.15\ \text{K}) = -2.95 \pm 1\ 07\ \text{kcal·mol}^{-1}$ and the drift 2.47 cal·K^{-1}·mol^{-1} (the 2nd law enthalpy of reaction being −8.62 kcal·mol^{-1}). Using the 3rd law $\Delta_r H°(298.15\ \text{K})$ and JANAF auxiliary data, we obtain $\Delta_f H°(\text{LiBO}_2, \text{g}, 298.15\ \text{K}) = -150.6\ \text{kcal·mol}^{-1}$. The uncertainty in this measurement is about 6 kcal·mol^{-1}.

Buchler and Berkowitz-Mattuck[2] studied mass spectrometrically the vaporization of lithium metaborate and reported $\Delta_{vap}H°(1160\ \text{K}) = 70 \pm 3\ \text{kcal·mol}^{-1}$ for LiBO$_2$(l) → LiBO$_2$(g) and $\Delta_{sub}H°(1060\ \text{K}) = 79 \pm 3\ \text{kcal·mol}^{-1}$ for LiBO$_2$(cr) → LiBO$_2$(g) by a 2nd law method. JANAF reduction to 298.15 K gives vap H(298.15 K) = 78.1 → 3 kcal·mol^{-1} and $\Delta_{sub}H°(298.15\ \text{K}) = 82.4 \pm 3\ \text{kcal·mol}^{-1}$. They also determined the vapor pressure of LiBO$_2$ at 1160 K as 2.0×10^{-6} atm by comparison with the vapor pressure of silver. JANAF 3rd law analysis of this single vapor pressure point gives $\Delta_{vap}H°(298.15\ \text{K}) = 85.0\ \text{kcal·mol}^{-1}$ which leads to $\Delta_f H°(\text{LiBO}_2, \text{g}, 298.15\ \text{K}) = -154.0 \pm 3\ \text{kcal·mol}^{-1}$. The latter is in good agreement with the value adopted in the tabulation. The 2nd law enthalpies of vaporization and sublimation are probably in error by about 6 kcal·mol^{-1}.

Hildenbrand *et al.*[3] measured the total vapor pressure over liquid LiBO$_2$ in the temperature range from 1120 to 1280 K by a torsion-effusion method. Assuming 100% monomeric vapor species, JANAF 3rd law analysis of their vapor pressure data yields the enthalpy of vaporization, $\Delta_{vap}H°(298.15\ \text{K}) = 84.47\ \text{kcal·mol}^{-1}$, and a drift of 0.93 ± 1.0 cal·K^{-1}·mol^{-1}, this corresponds to $\Delta_{sub}H°(298.15\ \text{K}) = 89.0\ \text{kcal·mol}^{-1}$. (2nd law heat of vaporization is $\Delta_{vap}H°(298.15\ \text{K}) = 83.25 \pm 1.20\ \text{kcal·mol}^{-1}$. Using the 3rd law $\Delta_{vap}H°(298.15\ \text{K})$, we obtain $\Delta_f H°(\text{LiBO}_2, \text{g}, 298.15\ \text{K}) = -154.6\ \text{kcal·mol}^{-1}$. If there are 10% of LiBO$_2$ dimer molecules present in the vapor phase as suggested by Buchler,[2] the correction in the 3rd law $\Delta_{vap}H°(298.15\ \text{K})$ is about 0.3 kcal·mol^{-1} is about 0.3 kcal·mol^{-1}which is much less than the uncertainty assigned to derive $\Delta_{vap}H°(298.15\ \text{K})$. The value, $\Delta_f H°(\text{LiBO}, \text{g}, 298.15\ \text{K}) = -154.6 \pm 3\ \text{kcal·mol}^{-1}$, is adopted in the tabulation.

Heat Capacity and Entropy

The adopted vibrational frequencies are obtained from Seshadri, Nimon and White[4] who observed the infrared spectra of LiBO$_2$ in an argon matrix and made a complete assignement of all six fundamentals. The uncertainty of the calculated statistical entropy at 298.15 K is estimated to be 1 cal·K^{-1}·mol^{-1} which is due to the magnitude of the matrix shifts from the free molecule spectrum, particularly for the lower frequency modes.

Buchler and Marram[5] observed only two vibrational frequencies, 1935 and 600 cm^{-1}, in their infrared spectra. These two frequencies are in reasonable agreement with those reported by Seshadri.[4]

By electron diffraction studies, Akishin and Spiridonov[6] determined the molecular structure of gaseous lithium metaborate and found the bond lengths and angles which are adopted in the tabulation. We tentatively select the bond angles Li-O-B as 90 from their reported data, i.e, 90-105 because Seshadri *et al.*[4] treated this bond angle as a parameter in the force constant calculations and found that the best fit to the infrared spectrometric data occurs at approximately 90. A recent electron diffraction study[7] on lithium metaborate confirms the results given by Akishin.[6]

The principal moments of inertia are $I_A = 2.5800 \times 10^{-39}$, $I_B = 11.0962 \times 10^{-39}$ and $I_C = 13.6763 \times 10^{-39}\ \text{g·cm}^2$.

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$\Delta_fH°(0\ K) = -247.99 \pm 1.55\ kJ\cdot mol^{-1}$
$S°(298.15\ K) = 14.795\ J\cdot K^{-1}\cdot mol^{-1}$ $\Delta_fH°(298.15\ K) = -250.91 \pm 1.55\ kJ\cdot mol^{-1}$
$T_{dcm} = 2600 \pm 100\ K$

Enthalpy of Formation

The adopted enthalpy of formation was determined by Wise *et al.*[5] using combustion in fluorine. Other recent calorimetric values are in good agreement as summarized below. Torsion effusion studies of the decomposition BN(cr) → B(am) + 0.5 $N_2(g)$ by Hildebrand and Hall[7] yield essentially the same $\Delta_fH°$ and indicate that the condensation coefficient $\alpha < 6 \times 10^{-3}$ for $N_2(g)$ on the surface of the sample. Use of $\alpha = 6 \times 10^{-3}$ brings the following decomposition studies into reasonable agreement. Langmuir studies by Dreger *et al.*,[8] mass spectrometric studies by Schissel and Williams;[9] and Knudsen effusion studies by Hoch and White.[10]

Source	Reaction	$\Delta_rH°(298.15\ K)$ kcal·mol^{-1}	$\Delta_fH°(298.15\ K)$ kcal·mol^{1}
1	$BN(cr) + 3/4\ O_2(g)\ 0.5\ B_2O_3(am) + 0.5\ N_2$	−90.1 ± 0.5	−59.7 ± 0.7
2	$B(am) + 0.5\ N_2(g) \rightarrow BN(cr)$	−60.8 ± 0.3	−59.6 ± 0.8
3	$BN(cr) + 1.5\ F_2(g) \rightarrow BF_3(g) + 0.5\ N_2$	−211.2 ± 0.1	
		−271.4	−60.2
4	$BN(cr) + NF_3(g) \rightarrow BF_3(g) + N_2$	−177.63 ± 0.3	
	$B(cr) + NF_3(g) \rightarrow BF_3(g) + 0.5\ N_2$	−237.77 ± 0.5	−60.1 ± 2
5	Combustion in O_2–H_2O	—	−59.9 ± 1.5
6	$BN(cr) + 1.5\ F_2(g) \rightarrow BF_3(g) + 0.5\ N_2$	−211.68 ± 0.3	−59.97 ± 0.37

Heat Capacity and Entropy

The low temperature heat capacity was taken from Westrum [11] The intermediate heat capacity (300–1650°C) was obtained from McDonald and Stull.[12] The high temperature C_p was taken from Prophet and Stull.[13] The heat capacities in the three temperature ranges were plotted and then graphically smoothed. Dworkin *et al.*[1] also reported that heat capacity (50–300 K) not employed in this table.

The entropy was obtained by integration of the heat capacity data from Westrum[11] based upon $S°(10\ K) = 0.0028\ cal\cdot K^{-1}mol^{-1}$.

Decomposition Data

Observations by the Dow Chemical Company under contract No. AF 33(616) 6194 show decomposition to elements at 1 atm total pressure at 2600 ± 100 K. The decomposition temperature calculated from these tables is 2832 K, presumably this discrepancy is associated with uncertainties in the high temperature enthalpies of BN(cr), B(cr), and B(l) and the enthalpy of melting of B(cr).

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−2.628	−247.993	−247.993	INFINITE
100	4.950	2.791	27.183	−2.439	−249.280	−241.538	126.166
200	12.414	8.473	16.359	−1.577	−250.206	−233.418	60.963
298.15	19.719	14.795	14.795	0.	−250.914	−225.022	39.423
300	19.849	14.917	14.795	0.037	−250.926	−224.861	39.152
400	26.276	21.539	15.654	2.354	−251.430	−216.091	28.219
500	31.380	27.974	17.480	5.247	−251.737	−207.217	21.648
600	35.229	34.051	19.741	8.586	−251.871	−198.298	17.263
700	38.074	39.701	22.194	12.255	−251.879	−189.367	14.131
800	40.459	44.943	24.714	16.184	−251.787	−180.442	11.782
900	42.593	49.836	27.236	20.339	−251.602	−171.534	9.956
1000	44.350	54.417	29.728	24.689	−251.334	−162.652	8.496
1100	45.815	58.716	32.170	29.201	−251.001	−153.799	7.303
1200	46.861	62.749	34.552	33.836	−250.629	−144.979	6.311
1300	47.698	66.534	36.868	38.566	−250.237	−136.190	5.472
1400	48.283	70.091	39.115	43.367	−249.844	−127.432	4.755
1500	48.702	73.438	41.293	48.218	−249.461	−118.702	4.134
1600	48.911	76.589	43.401	53.099	−249.105	−109.996	3.591
1700	48.939	79.555	45.442	57.992	−248.791	−101.312	3.113
1800	48.953	82.352	47.415	62.887	−248.526	−92.645	2.688
1900	48.953	84.999	49.324	67.782	−248.307	−83.991	2.309
2000	48.953	87.510	51.171	72.677	−248.134	−75.347	1.968
2100	48.953	89.899	52.959	77.573	−248.003	−66.711	1.659
2200	48.953	92.176	54 690	82.468	−247.915	−58.080	1.379
2300	48.953	94.352	56.368	87.363	−247.867	−49.453	1.123
2400	48.953	96.435	57.994	92.258	−298.118	−39.758	0.865
2500	48.953	98.434	59.572	97.154	−298.226	−28.990	0.606
2600	48.953	100.354	61.104	102.049	−298.339	−18.219	0.366
2700	48.953	102.201	62.592	106.944	−298.456	−7.443	0.144
2800	48.953	103.981	64 039	111.840	−298.578	3.338	−0.062
2900	48.953	105.699	65.446	116.735	−298.704	14.123	−0.254
3000	48.953	107.359	66.815	121.630	−298.834	24.912	−0.434
3100	48.953	108.964	68.149	126.525	−298.966	35.706	−0.602
3200	48.953	110.518	69.449	131.421	−299.103	46.504	−0.759
3300	48.953	112.024	70.717	136.316	−299.242	57 306	−0.907
3400	48.953	113.486	71.953	141.211	−299.384	68.113	−1.046
3500	48.953	114.905	73.160	146.107	−299.528	78.923	−1.178

PREVIOUS: March 1964 CURRENT: June 1966

$\Delta_fH°(0\ K) = 474 \pm 125\ kJ{\cdot}mol^{-1}$

$S°(298.15\ K) = 212.36\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298.15\ K) = 477 \pm 125\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
${}^3\Pi$	0	6
	[8500]	1
	[8900]	2
	27877	6

$\omega_e = 1514.6\ cm^{-1}$ $\omega_ex_e = 12.3\ cm^{-1}$ $\sigma = 1$

$B_e = 1.666\ cm^{-1}$ $\alpha_e = 0.025\ cm^{-1}$ $r_e = 1.281$ Å

Enthalpy of Formation

The enthalpy of formation is based on $D_0^\circ = 5.7$ eV which was calculated from ω_e and ω_ex_e observed by Douglas and Herzberg.[1] An uncertainty of ±1.3 eV was assigned from consideration of other information which places the dissociation energy between 4 and 7 eV. The value $D_0^\circ = 4.0 \pm 0.5$ eV was selected by Gaydon[2] from his own extrapolation of the spectroscopic data. An upper limit of $D_0^\circ < 7.0$ eV results from the upper limit for the pressure of BN(cr) → BN(g) obtained from the B^+ ion intensity at 1600°C observed by Akishin and Klodeev.[3] It is likely that the BN(g) pressure is even smaller since it is known that BN(cr) → B(s) + 0.5 N_2(g) and Akishin's pressure limit is the same magnitude as that of B(cr) → B(g). Fesenko[4] reports a standard enthalpy of sublimation of 160 kcal·mol^{-1} for BN(cr) → BN(g) and also gives pressures for BN(g) at 2500 and 3000 K which are stated to be two orders less than the equilibrium pressure of nitrogen. Fesenko's original article is not yet available to us and it is not clear from the abstract whether the values are based on new data or are merely calculations. The reported pressures yield $D_0^\circ = 6.2$ eV but here again the BN(g) pressures are of the same magnitude as the JANAF values for B(s) → B(g).

Some estimated values for D_0° (ranging from 5.4 to 6.4 eV) are summarized below along with the experimental evidence.

Source	D_0°(ev)	$\Delta_{sub}H°$(298.15 K), kcal·mol^{-1}	$\Delta_fH°$(298.15 K), kcal·mol^{-1}
Gaydon's extrapolation of spectroscopic data	4.0 ± 0.5	213	153
Linear Birge Sponer extrapolation	5.7	174	114
Fesenko's BN(g) pressures	6.2	161	101
Akishin's upper limit for BN(g) pressure	7.0	145	85
Estimate from geometric mean of $D°$ for B_2 and N_2	5.4	180	120
Estimate from $D°$ for series N_2, CN, BN, BeN	5.6	177	117
Estimate $M_2 + N_2 = 2$ MN for M=B from M=C	6.0	166	106
Estimate from arithmetic mean of $D°$ for B_2 and N_2	6.4	158	98

Heat Capacity and Entropy

The molecular constants are based on emission spectra of the ${}^3\Pi-{}^3\Pi$ transition otained by Douglas and Herzberg.[1] Observations of the same triplet in absorption by Thrush[5] strongly suggests that the ground state of BN is ${}^1\Pi$ in contrast to ${}^1\Sigma$ as observed for the isoelectronic molecules BeO and C_2. Electronic levels for the ${}^3\Pi$ states are taken from Douglas and Herzberg[1] while values for ${}^1\Sigma^+$ and ${}^1\Pi$ have been estimated from the SCF calculations of Masse and Barlochter.[6]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	-8.686	473.839	473.839	INFINITE
100	29.107	180.503	238.329	-5.783	475.267	465.238	-243.016
200	29.136	200.682	215.038	-2.871	476.391	454.736	-118.765
250	29.235	207 192	212.842	-1.412	476.751	449.278	-93.872
298.15	29.450	212.358	212.358	0.	476.976	443.965	-77.781
300	29.461	212.541	212.359	0.054	476.983	443.760	-77.265
350	29.820	217.107	212.719	1.536	477.108	438.212	-65.400
400	30.280	221.119	213.523	3.038	477.145	432.652	-56.499
450	30.797	224.715	214.570	4.565	477.111	427.091	-49.575
500	31.333	227.987	215.751	6.118	477.024	421.538	-44.038
600	32.362	233.792	218.286	9.304	476.737	410.465	-35.734
700	33.257	238.850	220.870	12.586	476.343	399.450	-29.807
800	34.001	243.341	223.403	15.950	475.870	388.497	-25.366
900	34.609	247.382	225.847	19.382	475.331	377.607	-21.916
1000	35.105	251.055	228.187	22.868	474.735	366.780	-19.159
1100	35.514	254.421	230.421	26.400	474.088	356.015	-16.906
1200	35.857	257.526	232.552	29.969	473.394	345.312	-15.031
1300	36.150	260.408	234.585	33.570	472.656	334.668	-13 447
1400	36 405	263.096	236.527	37.198	471.878	324.082	-12.092
1500	36.633	265.616	238.383	40.850	471.061	313.554	-10.919
1600	36 841	267.987	240.160	44.523	470.209	303.081	-9.895
1700	37.034	270.226	241.863	48.217	469.324	292.662	-8.992
1800	37.218	272.348	243.498	51.930	468.408	282.296	-8.192
1900	37.394	274.365	245.070	55.661	467.462	271.983	-7.477
2000	37.565	276.288	246.584	59.409	466.488	261.719	-6.835
2100	37.732	278.125	248.042	63.174	465.488	251.505	-6.256
2200	37.895	279.884	249.450	66.955	464.463	241.340	-5.730
2300	38.055	281.572	250.810	70.752	463.413	231.221	-5.251
2400	38.211	283.195	252.126	74.566	412.080	222.217	-4.836
2500	38.364	284.758	253.400	78.395	410.905	214.331	-4.478
2600	38.514	286.265	254.635	82.239	409.741	206.491	-4.148
2700	38.661	287.722	255.834	86.097	408.587	198.695	-3.844
2800	38.803	289 130	256.998	89.971	407.443	190.942	-3.562
2900	38.941	290.494	258.130	93.858	406.309	183.230	-3.300
3000	39.076	291.817	259.230	97.759	405.185	175.557	-3.057
3100	39.205	293.100	260.302	101.673	404.071	167.921	-2.829
3200	39.331	294.347	261.347	105.600	402.967	160.321	-2.617
3300	39.452	295.559	262.365	109.539	401.872	152.755	-2.418
3400	39.569	296.738	263.359	113.490	400.786	145.223	-2.231
3500	39.681	297.887	264.329	117.452	399.708	137.722	-2.055
3600	39.789	299.006	265.277	121.426	398.639	130.252	-1.890
3700	39.893	300.098	266.203	125.410	397.579	122.811	-1.734
3800	39.994	301.163	267.110	129.404	396.526	115.399	-1.586
3900	40.090	302.203	267.996	133.409	395.481	108.015	-1.447
4000	40.183	303.220	268.864	137.422	394.443	100.657	-1.314
4100	40.272	304.213	269.714	141.445	393.412	93.325	-1.189
4200	40.359	305.184	270.547	145.477	-87.461	93.043	-1.157
4300	40.442	306.135	271.364	149.517	-87.391	97.339	-1.182
4400	40.523	307.066	272.165	153.565	-87.317	101.635	-1.207
4500	40.602	307 977	272.950	157.621	-87.238	105.928	-1.230
4600	40.678	308.871	273.722	161.685	-87.156	110.220	-1.252
4700	40.752	309.746	274.479	165.757	-87.070	114.510	-1.273
4800	40.824	310.605	275.222	169.836	-86.982	118.798	-1.293
4900	40.894	311.447	275.953	173.922	-86.892	123.084	-1.312
5000	40.963	312.274	276.671	178.014	-86.800	127.368	-1.331
5100	41.031	313.086	277.377	182.114	-86.706	131.650	-1.348
5200	41.097	313.883	278.072	186.221	-86.612	135.931	-1.365
5300	41.163	314.667	278.755	190.334	-86.517	140.210	-1.382
5400	41.227	315.437	279.427	194.453	-86.422	144.487	-1.398
5500	41.291	316.194	280.089	198.579	-86.327	148.762	-1.413
5600	41.353	316.939	280.740	202.711	-86.233	153.035	-1.427
5700	41.416	317.671	281.382	206.850	-86.141	157.307	-1.442
5800	41.477	318.392	282.014	210.994	-86.051	161.578	-1.455
5900	41.538	319.101	282.636	215.145	-85.963	165.846	-1.468
6000	41.599	319.800	283.250	219.302	-85.878	170.113	-1.481

PREVIOUS June1966 (1 atm) CURRENT: June 1966 (1 bar)

Sodium Borate ($NaBO_2$) CRYSTAL $M_r = 65.79857$ **Sodium Borate ($NaBO_2$)** $B_1Na_1O_2(cr)$

$S°(298.15\ K) = 73.538 \pm 0.08\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 1240 \pm 2\ K$

$\Delta_f H°(0\ K) = -971.0 \pm 2.5\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -975.7 \pm 2.1\ kJ{\cdot}mol^{-1}$
$\Delta_{fus} H° = 33.47 \pm 2.0\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

Adami and Joe[1] measured enthalpies of solution of $B_2O_3(cr)$, $NaCl(cr)$ and $NaBO_2(cr)$ in aqueous HCl solution and derived $\Delta_r H°(298.15\ K) = -12.43 \pm 0.1\ kcal{\cdot}mol^{-1}$ for $NaBO_2(cr) + HCl(12.732\ H_2O,\ aq) \rightarrow NaCl(cr) + 1/2\ B_2O_3(cr) + 1/2\ H_2O(l)$ which leads to $\Delta_f H°(NaBO_2,\ cr,\ 298.15\ K) = -233.2 \pm 0.6\ kcal{\cdot}mol^{-1}$ using JANAF auxiliary data.[2] This value is adopted.

Grenier and White[3] measured the enthalpy of solution of crystal $Na_2OB_2O_3$ in 2N nitric acid solution at 0°C as $-20\ 43 \pm 0.36\ kcal\ mol^{-1}$. Since the correction term for $\Delta_{sol} H°$ from 0° to 25°C is generally small, we may assume the enthalpy of solution is the same at 0°C as at 25°C within the uncertainty of $\pm 1\ kcal{\cdot}mol^{-1}$. Thus we obtain $\Delta_{sol} H°(25°C) = -10.22 \pm 1\ kcal{\cdot}mol^{-1}$ for $NaBO_2(cr) + HNO_3(27.75\ H_2O,\ aq) + H_2O(l) \rightarrow NaNO_3(27.75\ H_2O,\ aq) + H_3BO_3(27.75\ H_2O,\ aq)$ from which we derived $\Delta_f H°(NaBO_2,\ cr,\ 298.15\ K) = -234.7 \pm 1.5\ kcal{\cdot}mol^{-1}$ based on JANAF auxiliary data.[4]

Shartsis and Capps[5] measured the heats of solution in 2N nitric acid of various Na_2O–B_2O_3 glass and crystalline mixtures containing 1.0–38.7 mole % of Na_2O. When their data are extrapolated to 50 mole %, we obtain $\Delta_{sol} H°(25°C) = -11.5 \pm 1.5\ kcal{\cdot}mol^{-1}$ for the same reaction as given before. The derived enthalpy of formation is $-233.4 \pm 1.5\ kcal{\cdot}mol^{-1}$ which is in good agreement with the value adopted.

Heat Capacity and Entropy

Grenier and Westrum[6] measured low temperature heat capacities from 5 to 346 K. The adopted C_p are derived from their experimental heat capacities by a polynomial curve fitting technique. The derived entropy, $S°(298.15\ K)$, is $17.576 \pm 0.02\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ based on $S° = 0.001\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ at 5.48 K. Pankratz[7] measured high temperature enthalpy data by drop calorimetry in the temperature range 404–1200.3 K. We adopt the smooth C_p derived by Pankratz. The average deviation of the observed enthalpy data from the adopted values is about 0.1%.

Fusion Data

Our analysis of several sets of binary phase data[8-10] yields the enthalpy of fusion, $\Delta_{fus} H° = 8.0 \pm 0.5\ kcal{\cdot}mol^{-1}$. Petit and Jaeger[11] derived $\Delta_{fus} H°(1239\ K) = 8.0\ kcal{\cdot}mol^{-1}$ from their phase data for the $NaBO_2$–NaF system. The adopted melting point (1240 K) is obtained from Pankratz.[7] Literature value include 1239 K,[8-12] 1238 K[13] and 1237 K.[14]

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	-11.634	-970.998	-970.998	INFINITE
100	32.430	20.000	123.003	-10.300	-973.933	-956.190	499.463
200	53.371	49.752	79.193	-5.888	-975.221	-937.851	244.942
298.15	65.940	73.538	73.538	0.	-975.709	-919.389	161.073
300	66.149	73.947	73.539	0.122	-975.714	-919.039	160.019
400	75.396	94.289	76.250	7.215	-978.576	-899.905	117.516
500	82.718	111.927	81.660	15.133	-978.549	-880.232	91.957
600	88.575	127.543	88.030	23.707	-978.132	-860.601	74.922
700	93.303	141.562	94.693	32.808	-977.394	-841.067	62.761
800	97.236	154.285	101.359	42.340	-976.390	-821.658	53.649
900	100.500	165.932	107.896	52.232	-975.173	-802.387	46.569
1000	103.219	176.667	114.244	62.423	-973.793	-783.262	40.913
1100	105.269	186 607	120.376	72.854	-972.310	-764.280	36.293
1200	106.608	195.831	126.284	83.456	-1067.556	-742.995	32.342
1240.000	106.859	199.331	128.584	87.726	--- CRYSTAL <--> LIQUID ---		
1300	107.320	204.391	131.967	94.151	-1065.165	-716.045	28.771
1400	108.127	212.374	137.429	104.923	-1062.774	-689.279	25.717
1500	108.935	219.861	142.677	115.776	-1060.375	-662.685	23.077
1600	109.742	226.917	147.724	126.710	-1057.963	-636.251	20.771
1700	110.549	233.595	152.580	137.724	-1055.536	-609.968	18.742
1800	111.356	239.936	157.259	148.820	-1053.090	-583.829	16.942
1900	112 162	245.979	161.770	159.996	-1050.624	-557.826	15.336
2000	112.968	251.752	166.126	171.252	-1048.138	-531.953	13.893

PREVIOUS: March 1965 CURRENT: June 1971

Sodium Borate ($NaBO_2$) $B_1Na_1O_2(cr)$

Sodium Borate ($NaBO_2$) LIQUID M_r = 65.79857 Sodium Borate (NaBO2) $B_1Na_1O_2(l)$

$S°(298.15\ K) = [82.958]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$T_{fus} = 1240 \pm 2\ K$

$\Delta_f H°(298.15\ K) = [-960.019]\ kJ{\cdot}mol^{-1}$

$\Delta_{fus} H° = 33.47 \pm 2.0\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(NaBO_2, l, 298.15\ K)$ is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(1240\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The constant heat capacity of the liquid is estimated to be 35 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ based on that of $LiBO_2(l)$, 34.491 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$,[1] which was derived from high temperature enthalpy measurements. A glass transition is assumed at 826 K below which the heat capacities are assumed to be the same as the crystal.

$S°(NaBO_2, l, 298.15\ K)$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

See the crystal table for details.

Vaporization Data

The boiling point is calculated as the temperature at which the fugacity is 1 bar for the reaction $NaBO_2(l) \rightarrow NaBO_2(g)$. The enthalpy of vaporization is the difference in $\Delta_f H°$ at the boiling point between liquid and gas.

Reference

[1] JANAF Thermochemical Table: $LiBO_2(l)$, 6–30–71.

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	65.940	82.958	82.958	0.	−960.019	−906.507	158.816
300	66.149	83.366	82.959	0.122	−960.024	−906.175	157.779
400	75.396	103.708	85.670	7.215	−962.886	−887.983	115.959
500	82.718	121.346	91.080	15.133	−962.859	−869.251	90.810
600	88.575	136.962	97.450	23.707	−962.442	−850.563	74.048
700	93.303	150.981	104.113	32.808	−961.704	−831.971	62.082
800	97.236	163.706	110.779	42.342	−960.699	−813.504	53.116
826.000	98.129	166.830	112.494	44.881	GLASS <––> LIQUID TRANSITION		
826 000	146.440	166.830	112.494	44.881			
900	146.440	179.395	117.486	55.718	−955.997	−795.328	46.160
1000	146.440	194.824	124.462	70.362	−950.164	−777.790	40.628
1100	146.440	208.781	131.503	85.006	−944.468	−760.829	36.129
1200	146.440	221.523	138.481	99.650	−1035.672	−741.941	32.296
1240.000	146.440	226.325	141.238	105.508	––– CRYSTAL <––> LIQUID –––		
1300	146.440	233.244	145.326	114.294	−1029.331	−717.722	28.838
1400	146.440	244.097	151.998	128.938	−1023.069	−693.987	25.893
1500	146.440	254.200	158.479	143.582	−1016.879	−670.698	23.356
1600	146.440	263.651	164.760	158.226	−1010.757	−647.819	21.149
1700	146.440	272.529	170.841	172.870	−1004.700	−625.321	19.214
1800	146.440	280.899	176.725	187.514	−998.706	−603.178	17.504
1900	146.440	288.817	182.418	202.158	−992.772	−581.366	15.983
2000	146.440	296.328	187.927	216.802	−986.898	−559.866	14.622
2100	146.440	303.473	193.261	231.446	−981.083	−538.657	13.398
2200	146.440	310.285	198.426	246.090	−975.327	−517.724	12.292
2300	146 440	316.795	203.432	260.734	−969.629	−497.052	11.288
2400	146.440	323.027	208.287	275.378	−1014.248	−475.558	10.350
2500	146.440	329.005	212.997	290.022	−1008.744	−453.225	9.470

PREVIOUS: March 1965   CURRENT: June 1971

Sodium Borate ($NaBO_2$) CRYSTAL-LIQUID

0 to 1240 K crystal
above 1240 K liquid

Refer to the individual tables for details.

M_r = 65.79857 Sodium Borate ($NaBO_2$) $B_1Na_1O_2(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−11.634	−970.998	−970.998	INFINITE
100	32.430	20.000	123.003	−10.300	−973.933	−956.190	499.463
200	53.371	49.752	79.193	−5.888	−975.221	−937.851	244.942
298.15	65.940	73.538	73.538	0.	−975.709	−919.389	161 073
300	66.149	73.947	73.539	0.122	−975.714	−919.039	160.019
400	75.396	94.289	76.250	7.215	−978.576	−899.905	117.516
500	82.718	111.927	81.660	15.133	−978.549	−880.232	91.957
600	88.575	127.543	88.030	23.707	−978.132	−860.601	74 922
700	93.303	141.562	94.693	32.808	−977.394	−841.067	62.761
800	97.236	154.285	101.359	42.340	−976.390	−821.658	53.649
900	100.500	165.932	107.896	52.232	−975.173	−802.387	46.569
1000	103.219	176.667	114.244	62.423	−973.793	−783.262	40.913
1100	105.269	186.607	120.376	72.854	−972.310	−764.280	36.293
1200	106.608	195.831	126.284	83.456	−1067.556	−742.995	32.342
1240.000	106.859	199.331	128.584	87.726	____ CRYSTAL <− −> LIQUID ____		
1240.000	146.440	226.325	128.584	121.198	TRANSITION		
1300	146.440	233.244	133.256	129.984	−1029.331	−717.721	28.838
1400	146.440	244 097	140.791	144.628	−1023.069	−693.986	25.893
1500	146.440	254.200	148.019	159.272	−1016.879	−670.697	23.356
1600	146.440	263.651	154.953	173.916	−1010.757	−647.818	21.149
1700	146.440	272.529	161.611	188.560	−1004 700	−625.321	19.214
1800	146.440	280.899	168.008	203.204	−998 705	−603.178	17.504
1900	146 440	288.817	174.160	217.848	−992.772	−581.366	15.983
2000	146.440	296.328	180.082	232.492	−986.898	−559.865	14.622
2100	146.440	303.473	185.789	247.136	−981.083	−538.657	13.398
2200	146.440	310.285	191.294	261.780	−975.326	−517.723	12.292
2300	146.440	316.795	196.610	276.424	−969.628	−497.052	11.288
2400	146.440	323.027	201 749	291.068	−1014.248	−475.557	10.350
2500	146.440	329.005	206.720	305.712	−1008.744	−453.225	9.470

PREVIOUS: CURRENT June 1971

Sodium Borate ($NaBO_2$) IDEAL GAS M_r = 65.79857 Sodium Borate ($NaBO_2$) $B_1Na_1O_2(g)$

$S°(298.15\ K) = 287.2 \pm 4.2\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = -645.9 \pm 12.6\ kJ{\cdot}mol^{-1}$

$\Delta_fH°(298.15\ K) = -648.5 \pm 12.6\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}
1960(1)	573(1)
1087(1)	363(1)
576(1)	108(1)

Ground State Quantum Weight: 1 $\sigma = 1$

Point Group: C_s

Bond Distances: Na–O = 2.14 Å; O–B = 1.36 Å; B=O = 1.20 Å

Bond Angles: Na–O–B = 90°; O–B–O = 180°

Product of the Moments of Inertia: $I_AI_BI_C = 2.407470 \times 10^{-114}\ g^3{\cdot}cm^6$

Enthalpy of Formation

Jensen[1] determined equilibrium constants for the reaction: $Na(g) + HBO_2(g) \rightarrow NaBO_2(g) + H(g)$ by flame studies. This technique involved several assumptions, the most basic of which was that boron added to $H_2/N_2/O_2$ flames was converted completely to HBO_2. The hydrogen atom concentration was taken from previous studies on such flames. Sodium metaborate was assumed to be formed in the flame. The concentration of Na atom was determined by atomic absorption spectrophotometry. JANAF 3rd law analysis of his equilibrium constant equation in the temperature range from 2000 to 2600 K yields $\Delta_rH(298.15\ K) = 7.55 \pm 1.08\ kcal{\cdot}mol^{-1}$ and the drift $2.50\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. (The 2nd law enthalpy of reaction is $\Delta_rH°(298.15\ K) = 1.81\ kcal{\cdot}mol^{-1}$.) Using the 3rd law $\Delta_rH°(298.15\ K)$ and JANAF auxiliary data, we obtain $\Delta_fH°(NaBO_2,\ g,\ 298.15\ K) = -152.8\ kcal{\cdot}mol^{-1}$. The uncertainty in this result is about $\pm 6\ kcal{\cdot}mol^{-1}$.

Buchler and Berkowitz–Mattuck[2] studied mass spectrometrically the sublimation of sodium metaborate and obtained $\Delta_{sub}H°(1070\ K) = 73 \pm 3\ kcal\ mol^{-1}$ for $NaBO_2(cr) \rightarrow NaBO_2(g)$ by a 2nd law method. JANAF reduction to 298.15 K gives $\Delta_{sub}H°(298.15\ K) = 76.6 \pm 3\ kcal{\cdot}mol^{-1}$ which leads to $\Delta_fH°(298.15\ K)(NaBO_2,\ g) = -156.6 \pm 3\ kcal{\cdot}mol^{-1}$. They also determined the vapor pressure of $NaBO_2$ at 1070 K as 5×10^{-7} atm by comparison with the vapor pressure of silver. JANAF 3rd law analysis of this single vapor pressure point gives $\Delta_{sub}H°(298.15\ K) = 83.37\ kcal{\cdot}mol^{-1}$ which leads to $\Delta_fH°(NaBO_2,\ g,\ 298.15\ K) = -149.8\ kcal{\cdot}mol^{-1}$.

Cole and Taylor[3] determined the vapor pressures of $NaBO_2(g)$ by a dynamic method with dry N_2 as carrier gas. Their vapor pressure data were taken over a flow–rate range where the apparent vapor pressure increased with decreasing flow rate, and the data were then extrapolated to zero flow rate. The vapor species of the sample was also assumed to be monomeric $NaBO_2(g)$. JANAF 3rd law analyses of their reported vapor pressure data over the liquid $NaBO_2$ in the temperature range 1150°C–1350°C yield $\Delta_{vap}H°(298.15\ K) = 75.37 \pm 3.32\ kcal{\cdot}mol^{-1}$ and the drift $-20.6\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. (The 2nd law enthalpy of vaporization is $\Delta_{vap}H°(298.15\ K) = 107\ kcal{\cdot}mol^{-1}$). Using the 3rd law $\Delta_{vap}H°(298.15\ K)$, we obtain $\Delta_fH°(298.15\ K) = -154.1 \pm 4\ kcal{\cdot}mol^{-1}$.

A weighted average, $\Delta_fH°(NaBO_2,\ g,\ 298.15\ K) = -155 \pm 3\ kcal{\cdot}mol^{-1}$, is adopted in the tabulation.

Heat Capacity and Entropy

The adopted vibrational frequencies are obtained from Seshadri *et al.*,[4] who observed the infrared spectra of $NaBO_2$ in an argon matrix and made a complete assignment of all six fundamentals. The uncertainty of the calculated statistical entropy at 298.15 K is estimated to be ±1 $cal{\cdot}mol^{-1}\ K^{-1}$ which is due to the magnitude of the matrix shifts from the free molecule spectrum, particularly for the lower frequency modes.

Buchler and Marran[5] observed only two vibrational frequencies, 1935 and 600 cm^{-1}, in their gas–phase infrared spectra. These two frequencies are in reasonable agreement with those reported by Seshadri.[4]

By electron diffraction studies, Akishin and Spiridonov[6] determined the molecular structure of gaseous sodium metaborate and found the bond length and angles which are adopted in the tabulation. The angle Na–O–B is taken as 90° based on that of $LiBO_2(g)$.[7]

The three principal moments of inertia are $I_A = 5.1904 \times 10^{-39}$, $I_B = 19.0974 \times 10^{-39}$, and $I_C = 24.2878 \times 10^{-39}\ g{\cdot}cm^2$.

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[7] JANAF Thermochemical Tables: $LiBO_2(g)$, 6–30–71.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	-13.703	-645.879	-645.879	INFINITE
100	41.612	233.779	333.819	-10.004	-646.448	-650.083	339.569
200	50.926	265.464	292.357	-5.379	-647.523	-653.295	170.623
250	54.980	277.277	288.189	-2.728	-648.025	-654.680	136.788
298.15	58.233	287.248	287.248	0.	-648.520	-655.918	114.914
300	58.346	287.608	287.249	0.108	-648.540	-655.964	114.213
350	61.142	296.819	287.970	3.097	-649.107	-657.157	98.075
400	63.496	305.141	289.604	6.215	-652.388	-658.058	85.934
450	65.510	312.739	291.759	9.441	-653.069	-658.726	76.463
500	67.255	319.734	294.211	12.761	-653.733	-659.318	68.879
600	70.125	332.261	299.533	19.636	-655.015	-660.314	57.485
700	72.365	343.246	305.009	26.765	-656.247	-661.100	49.332
800	74.131	353.029	310.412	34.094	-657.448	-661.711	43.205
900	75.536	361.844	315.645	41.580	-658.636	-662.172	38.431
1000	76.662	369.863	320.672	49.192	-659.836	-662.501	34.605
1100	77.572	377.214	325.482	56.905	-661.070	-662.708	31.469
1200	78.314	383.996	330.079	64.700	-759.123	-660.360	28.745
1300	78.924	390.290	334.472	72.563	-759.563	-652.112	26.202
1400	79.431	396.158	338.671	80.482	-760.027	-643.830	24.022
1500	79.855	401.653	342.688	88.446	-760.516	-635.513	22.131
1600	80.212	406.818	346.537	96.450	-761.034	-627.163	20.475
1700	80.517	411.690	350.227	104.487	-761.584	-618.779	19.013
1800	80.777	416.300	353.771	112.552	-762.169	-610.363	17.712
1900	81.002	420.674	357.178	120.641	-762.790	-601.912	16.548
2000	81.196	424.834	360.458	128.752	-763.450	-593.428	15.499
2100	81.366	428.799	363.619	136.880	-764.150	-584.910	14.549
2200	81.515	432.588	366.668	145.024	-764.894	-576.357	13.684
2300	81.647	436.215	369.614	153.182	-765.681	-567.770	12.894
2400	81.763	439.692	372.462	161.353	-816.774	-558.079	12.146
2500	81.866	443.032	375.218	169.535	-817.733	-547.280	11.435
2600	81.959	446.244	377.888	177.726	-818.708	-536.443	10.777
2700	82.042	449.339	380.478	185.926	-819.700	-525.567	10.168
2800	82.116	452.324	382.991	194.134	-820.711	-514.655	9.601
2900	82.184	455.207	385.431	202.349	-821.743	-503.707	9.073
3000	82.245	457.994	387.804	210.570	-822.798	-492.722	8.579
3100	82.300	460.692	390.112	218.798	-823.876	-481.701	8.117
3200	82.351	463.306	392.359	227.030	-824.979	-470.646	7.683
3300	82.397	465.840	394.547	235.268	-826.107	-459.556	7.274
3400	82.439	468.301	396.680	243.509	-827.264	-448.431	6.889
3500	82.478	470.691	398.761	251.755	-828.451	-437.272	6.526
3600	82.513	473.015	400.791	260.005	-829.668	-426.078	6.182
3700	82.546	475.276	402.774	268.258	-830.919	-414.851	5.857
3800	82.577	477.478	404.711	276.514	-832.205	-403.588	5.548
3900	82.605	479.623	406.605	284.773	-833.527	-392.291	5.254
4000	82.631	481.715	408.456	293.035	-834.889	-380.960	4.975
4100	82.655	483.756	410.268	301.299	-836.292	-369.595	4.709
4200	82.678	485.748	412.042	309.566	-1317.585	-351.171	4.367
4300	82.699	487.694	413.779	317.835	-1317.991	-328.156	3.986
4400	82.719	489.595	415.480	326.106	-1318.406	-305.135	3.622
4500	82.737	491.454	417.148	334.379	-1318.893	-282.102	3.275
4600	82.754	493.273	418.783	342.653	-1319.443	-259.056	2.942
4700	82.771	495.053	420.387	350.930	-1320.051	-235.998	2.623
4800	82.786	496.796	421.961	359.207	-1320.719	-212.926	2.317
4900	82.800	498.503	423.505	367.487	-1321.451	-189.839	2.024
5000	82.814	500.176	425.022	375.767	-1322.243	-166.737	1.742
5100	82.826	501.816	426.512	384.049	-1323.111	-143.618	1.471
5200	82.838	503.424	427.976	392.333	-1324.054	-120.483	1.210
5300	82.850	505.002	429.414	400.617	-1325.075	-97.327	0.959
5400	82.860	506.551	430.828	408.903	-1326.178	-74.152	0.717
5500	82.870	508.071	432.219	417.189	-1327.366	-50.956	0.484
5600	82.880	509.565	433.587	425.477	-1328.643	-27.736	0.259
5700	82.889	511.032	434.933	433.765	-1330.012	-4.494	0.041
5800	82.898	512.473	436.257	442.054	-1331.478	18.774	-0.169
5900	82.906	513.890	437.561	450.345	-1333.043	42.066	-0.372
6000	82.914	515.284	438.845	458.636	-1334.552	65.369	-0.569

PREVIOUS: June 1971 (1 atm) CURRENT: June 1971 (1 bar)

Boron Oxide (BO) **IDEAL GAS** M_r = 26,8094 **Boron Oxide (BO)** $B_1O_1(g)$

$S°(298.15\ K) = 203.47 \pm 0.04\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = -3.1 \pm 8\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 0 \pm 8\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$X^2\Sigma^+$	0	2
$A^2\Pi$	23836	2
$A^2\Pi$	23959	2
$B^2\Sigma$	39957	2
$B^2\Sigma^+$	43175	2

$\omega_e = 1895.66\ cm^{-1}$ $\omega_e x_e = 11.90\ cm^{-1}$ $\sigma = 1$
$B_e = 1.800\ cm^{-1}$ $\alpha_e = 0.01676\ cm^{-1}$ $r_e = 1.2049\ Å$

Enthalpy of Formation

The enthalpy of formation has recently been determined by several workers whose values are in close agreement. Blackburn, *et al.*[1] measured the ion currents corresponding to BO^+ and $B_2O_2^+$ as a function of temperature in a mass spectrometer. From a least squares fit of the data they report $\Delta H = 56.6 \pm 1.8$ kcal·mol^{-1} for the reaction $1/2B_2O_2(g) \rightarrow BO(g)$; this yields $\Delta_f H°$(BO, g, 298.15 K) = 2.1 ± 2.8 kcal·mol^{-1} using $\Delta_f H°(B_2O_2$, g, 298.15 K) = −109 ± 2 kcal·mol^{-1}.

De Galan, *et al.*[2] from flame photometric measurements reports $D_0°$(BO) = 8.3eV(191 4 kcal·mol^{-1}), which corresponds to $\Delta_f H°$(BO, g, 298.15 K) = −0.1 kcal·mol^{-1}.

Coppens, *et al.*[3] from a mass spectometric study of several isomolecular exchange reactions, conclude that $D_0°$(BO) = 8.29 ± 0.1 eV(191.2 ± 2.3 kcal·mol^{-1}) or $\Delta_f H°$(BO, g, 298.15 K) = 0.1 ± 2.3 kcal·mol^{-1}.

Farber, *et al.*[4] investigated the same reaction as Blackburn *et al.* and reported $\Delta_r H°$(1800 K) = 53 8 ± 1.9 kcal·mol^{-1}, which yields $\Delta_f H°$(BO, g, 298.15 K) = 0.9 ± 2.9 kcal·mol^{-1}.

We adopt a median value of 0 ± 2 kcal·mol^{-1} which includes all the determinations

Heat Capacity and Entropy

The molecular and vibrational constants for the ground state are from Herzberg.[5] The electronic levels are also given by Herzberg with the exception of the level at 39957, the $A^2\Sigma$ level designated B' by Mal'tsev and Kataev.[6] The molecular constants were all adjusted to reflect normal isotopic abundancies.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−8.674	−3.118	−3.118	INFINITE
100	29.105	171.662	229.370	−5.771	−1.692	−10.162	5.308
200	29.112	191.838	206.138	−2.860	−0.569	−19.105	4.990
250	29.133	198.336	203.952	−1.404	−0.213	−23.783	4.969
298.15	29 196	203.472	203.472	0.	0.	−28.343	4.966
300	29.200	203.652	203.472	0.054	0.006	−28.519	4.966
350	29.343	208.163	203.828	1.517	0.104	−33.283	4.967
400	29.574	212.096	204.621	2.990	0.094	−38.053	4.969
450	29.882	215.596	205.649	4.476	−0.007	−42.816	4.970
500	30.250	218.763	206.805	5.979	−0.178	−47.564	4.969
600	31.076	224.350	209.276	9.045	−0.673	−56.997	4.962
700	31.910	229.204	211.783	12.194	−1.306	−66.336	4.950
800	32.677	233.516	214.235	15.425	−2.027	−75.578	4.935
900	33.350	237.404	216.597	18.727	−2.809	−84.725	4.917
1000	33.926	240.949	218.858	22.091	−3.638	−93.783	4.899
1100	34.415	244.206	221.016	25.509	−4.505	−102.756	4.879
1200	34 829	247.219	223.075	28.972	−5.405	−111.648	4.860
1300	35.181	250.021	225.042	32.473	−6.337	−120.464	4.840
1400	35.481	252.639	226.920	36.006	−7.300	−129.208	4.821
1500	35.739	255.096	228.718	39.568	−8.294	−137.881	4.801
1600	35.961	257.410	230.439	43.153	−9.318	−146.487	4.782
1700	36.155	259.596	232.091	46.759	−10.375	−155.028	4.763
1800	36.324	261.667	233.677	50.383	−11.463	−163.505	4.745
1900	36.473	263.635	235.202	54.023	−12.584	−171.922	4.726
2000	36.606	265.510	236.671	57.677	−13.739	−180.278	4.708
2100	36.724	267.299	238.087	61.344	−14.928	−188.576	4.691
2200	36.831	269.010	239.454	65.022	−16.151	−196.816	4.673
2300	36.928	270.649	240.775	68.710	−17.409	−205.000	4.656
2400	37.016	272.222	242.053	72.407	−68.961	−212.060	4.615
2500	37.098	273.735	243.290	76.113	−70.368	−217.994	4.555
2600	37.173	275.192	244.489	79.826	−71.778	−223.871	4.498
2700	37.244	276.596	245.653	83.547	−73.190	−229.694	4.444
2800	37.310	277.952	246.782	87.275	−74.607	−235.464	4.393
2900	37.374	279.262	247.880	91.009	−76.026	−241.185	4.344
3000	37.435	280.530	248.947	94.749	−77.449	−246.855	4.298
3100	37.495	281.759	249.986	98.496	−78.876	−252.478	4.254
3200	37.554	282.950	250.997	102.248	−80.305	−258.056	4.212
3300	37.613	284.106	251.983	106.007	−81.737	−263.589	4.172
3400	37.672	285.230	252.945	109.771	−83.172	−269.078	4.134
3500	37.731	286.323	253.883	113.541	−84.609	−274.525	4.097
3600	37.792	287.387	254.799	117.317	−86.047	−279.930	4.062
3700	37.855	288.423	255.693	121.100	−87.487	−285.296	4.028
3800	37.920	289.433	256.568	124.888	−88.927	−290.623	3.995
3900	37.987	290.419	257.424	128.684	−90.368	−295.912	3.963
4000	38.057	291.382	258.261	132.486	−91.809	−301.164	3.933
4100	38.130	292.323	259.080	136.295	−93.249	−306.380	3.903
4200	38.206	293.242	259.882	140.112	−574.537	−304.537	3.787
4300	38.285	294.142	260.669	143.936	−574.887	−298.104	3.621
4400	38.368	295.023	261.439	147.769	−575.237	−291.663	3.462
4500	38.455	295.887	262.195	151.610	−575.586	−285.215	3.311
4600	38.546	296.733	262.937	155.460	−575.935	−278.758	3.165
4700	38 640	297.563	263.665	159.319	−576.284	−272.294	3.026
4800	38.738	298.377	264.380	163.188	−576.632	−265.823	2.893
4900	38.840	299.177	265.082	167.067	−576.980	−259.343	2.765
5000	38.946	299.963	265.771	170.956	−577.327	−252.858	2.642
5100	39.055	300.735	266.449	174.856	−577.674	−246.365	2.523
5200	39.169	301.495	267.116	178.768	−578.020	−239.865	2.409
5300	39.285	302.242	267.772	182.690	−578.368	−233.359	2.300
5400	39.406	302.977	268.417	186.625	−578.715	−226.846	2.194
5500	39.529	303.701	269.052	190.571	−579.064	−220.327	2.092
5600	39.656	304.415	269.677	194.531	−579.414	−213.801	1.994
5700	39.787	305.118	270.293	198.503	−579.766	−207.269	1.899
5800	39.920	305.811	270.899	202.488	−580.120	−200.731	1.808
5900	40.055	306.494	271.497	206.487	−580.477	−194.187	1.719
6000	40.194	307.169	272.086	210.499	−580.838	−187.637	1.634

PREVIOUS June 1968 (1 atm) CURRENT. June 1968 (1 bar)

Boron Oxide (BO) $B_1O_1(g)$

Boron Oxide (BO$_2$) IDEAL GAS $M_r = 42.8088$ Boron Oxide (BO$_2$) B$_1$O$_2$(g)

$S°(298.15\ K) = 229.81 \pm 0.20\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -285 \pm 8\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -285 \pm 8\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^2\Pi_g$	0	2
$^2\Pi_g$	1.49	2
$^2\Pi_u$	18291.6	4
$^2\Sigma_u^+$	24508.0	2

Vibrational Frequencies and Degeneracies
ν, cm^{-1}

1056 (1)
454 (2)
1321.7 (1)

Point Group: $D_{\infty h}$ $\sigma = 2$
Bond Distance: B–O = 1.263 Å
Bond Angle: O–B–O = 180°
Rotational Constant : $B_0 = 0.33026$ cm^{-1}

Enthalpy of Formation

Greene[1] measured the vapor pressure of B_2O_3 and examined the infrared absorption spectra of B_2O_3, B_2O_2 and BO_2. The isotope shift and oxygen and temperature dependencies of the boric acid fluctuation bands were studied. The enthalpy change, $\Delta_r H°(2100\ K) = 76 \pm 2$ kcal·mol^{-1}, for the reaction $1/2\ B_2O_3(l) + 1/4\ O_2(g) = BO_2(g)$, was obtained spectroscopically. Based on this data and $\Delta_f H°(B_2O_3,\ l,\ 2100\ K) = -291.05$ kcal·mol^{-1}, we derive $\Delta_f H°(BO_2,\ g,\ 298.15\ K) = -68.4 \pm 2$ kcal·mol^{-1}.

Rusin[2] determined the equilibrium constant of the reaction $HBO_2(g) + OH(g) = BO_2(g) + H_2O(g)$ by simultaneously recording the pressure and spectra at 3000–3200 K of HBO_2 and BO_2, which were produced from the combustion in a bomb of mixtures of H, O, CO and a small amount of B_2H_6. Using the experimental value $K_p(3100\ K) = 0.9$, and JANAF Gibbs energy functions for the reactants and products, we obtain $\Delta_r H°(298.15\ K) = 0.53$ kcal·mol^{-1} for that reaction. Employing $\Delta_f H°(298.15\ K) = -134.00$, 9.43 and -57.80 kcal·mol^{-1} for $HBO_2(g)$, OH(g) and $H_2O(g)$, respectively, we derive the value $\Delta_f H°(BO_2,\ g,\ 298.15\ K) = -66.24$ kcal·mol^{-1}.

In a study of gases from flames containing trimethylborate stabilized on flat porous metal burners, Kaskan[3] obtained data consistent with the bands being due to the molecule $BO_2(g)$. The temperature dependence of the equilibrium constants for the reaction $OH(g) + HBO_2(g) = H_2O(g) + BO_2(g)$ was investigated and the data were reported to be consistent with a value $\Delta_r H°(1800\ K) = -16$ kcal·mol^{-1}. Based on this $\Delta_r H°(1800\ K)$ value, we calculate $\Delta_f H°(BO_2,\ g,\ 298.15\ K) = -83.62$ kcal·mol^{-1}. Kaskan[4] has studied the effect of oxygen on the intensity of absorption (5470 Å) in the green or "fluctuation" bands of the gas phase in equilibrium with $B_2O_3(l)$. At constant temperature the absorptivity was found to depend on the 1/4 power of the oxygen pressure. This is interpreted as evidence that the absorbing species is $BO_2(g)$. The reaction $1/2\ B_2O_3(l) + 1/4\ O_2(g) = BO_2(g)$ was found to be 70 kcal·mol^{-1} *endothermic in the temperature range* 1660–1950 K, yielding $\Delta_f H°(BO_2,\ g,\ 298.15\ K) = -75.28$ kcal·mol^{-1}. Rusin *et al.*[2] discussed the discrepancy between their results and those of the above two investigations and commented that the results of Kaskan[3] [4] were derived based on the assumption that Beer's law was obeyed over the temperature range 1400–2200 K. Actually, the relative population α of the principal electronic state $X^2\Pi$ of the BO_2 molecule changes greatly over this temperature range Therefore the expression for the dependence of the optical density on the concentration of BO_2 must be corrected to allow for the variation of α with temperature.

The enthalpy of formation of $BO_2(g)$ at 298.15 K is selected as -68 ± 2 kcal·mol^{-1}.

Heat Capacity and Entropy

The electronic levels and quantum weights are obtained from Johns.[5] Vibrational frequencies, bond distance and rotational constant were reported by Johns,[5] Sommer,[6] and Snowden.[7] The values adopted are those determined by Snowden.[7] Snowden used a (1 1) mixture of KBF_4 and B_2O_3 placed in a 13 mm Vycor tube. The mixture was heated to produce a vapor which passed through an external electrodeless discharge. The intense emission spectrum of the BO_2 molecule was observed. The fluorescence spectrum obtained by Johns was too weak for a full characterization of the electronic ground state.

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−10.731	−285.346	−285.346	INFINITE
100	33.725	188.764	264.960	−7.620	−285.163	−286.678	149.745
200	38.528	213.526	233.623	−4.019	−284.807	−288.331	75.304
250	41.020	222.394	230.514	−2.030	−284.646	−289.231	60.432
298.15	43.276	229.814	229.814	0.	−284.512	−290.127	50.829
300	43.359	230.082	229.815	0.080	−284.507	−290.162	50.522
350	45.527	236.931	230.351	2.303	−284.388	−291.114	43.446
400	47 495	243.141	231.567	4.630	−284.292	−292.082	38.142
450	49.246	248.838	233.174	7.049	−284.217	−293.060	34.018
500	50.780	254.108	235.007	9.550	−284.160	−294.046	30.719
600	53.263	263.597	238.999	14.759	−284.093	−296.030	25.772
700	55.110	271.953	243.122	20.182	−284.080	−298.021	22.239
800	56.490	279.406	247.200	25.765	−284.116	−300.011	19.589
900	57.533	286.123	251.158	31.469	−284.200	−301.994	17.527
1000	58.333	292.228	254.964	37.264	−284.329	−303.964	15.877
1100	58.957	297.818	258.610	43.129	−284.502	−305.920	14.527
1200	59.451	302.970	262.094	49.051	−284.719	−307.857	13.401
1300	59.847	307.745	265.425	55.016	−284.978	−309.776	12.447
1400	60.169	312.192	268.608	61.018	−285.280	−311.672	11.629
1500	60.435	316.353	271.654	67.048	−285.624	−313.546	10.919
1600	60.655	320.260	274.571	73.103	−286.013	−315.395	10.297
1700	60.841	323.943	277.368	79.178	−286.446	−317.218	9.747
1800	60.998	327.425	280.053	85.270	−286.924	−319.015	9.258
1900	61.133	330.727	282.634	91.377	−287.449	−320.783	8.819
2000	61.250	333.866	285.118	97.496	−288.019	−322.523	8.423
2100	61.352	336.857	287.511	103.627	−288.637	−324.233	8.065
2200	61.443	339.713	289.819	109.766	−289.302	−325.912	7.738
2300	61.523	342.446	292.048	115.915	−290.016	−327.561	7.439
2400	61.597	345.066	294.203	122.071	−341.036	−328.109	7.141
2500	61.664	347.582	296.288	128.234	−341.923	−327.552	6.844
2600	61.728	350.002	298.308	134.404	−342.824	−326.959	6.569
2700	61.788	352.332	300.266	140.579	−343.741	−326.332	6.313
2800	61.847	354.581	302.166	146.761	−344.672	−325.670	6.075
2900	61.904	356.752	304.011	152.949	−345.617	−324.975	5.853
3000	61.961	358.852	305.804	159.142	−346.575	−324.247	5.646
3100	62.019	360.884	307.548	165.341	−347.547	−323.486	5.451
3200	62.078	362.854	309.246	171.546	−348.531	−322.695	5.267
3300	62.138	364.765	310.900	177.757	−349.526	−321.872	5.095
3400	62.201	366.621	312.511	183.974	−350.532	−321.019	4.932
3500	62.265	368.425	314.083	190.197	−351.548	−320.136	4.778
3600	62.333	370.180	315.617	196.427	−352.572	−319.224	4.632
3700	62.403	371.889	317.115	202.663	−353.604	−318.284	4.493
3800	62.475	373.554	318.579	208.907	−354.644	−317.315	4.362
3900	62.551	375.178	320.009	215.159	−355.690	−316.318	4.237
4000	62.629	376.763	321.408	221.418	−356.741	−315.296	4.117
4100	62.711	378.310	322.777	227.685	−357.798	−314.247	4.004
4200	62.795	379.822	324.117	233.960	−838.708	−306.148	3.808
4300	62.882	381.301	325.430	240.244	−838.686	−293.467	3.565
4400	62.971	382.747	326.716	246.536	−838.669	−280.789	3.333
4500	63.062	384.164	327.977	252.838	−838.657	−268.110	3.112
4600	63.156	385.551	329.214	259.149	−838.650	−255.432	2.901
4700	63.252	386.910	330.427	265.469	−838.649	−242.753	2.698
4800	63.350	388.243	331.618	271.799	−838.653	−230.074	2.504
4900	63.449	389.550	332.787	278.139	−838.664	−217.395	2.317
5000	63.549	390.833	333.935	284.489	−838.680	−204.715	2.139
5100	63.651	392.092	335.063	290.849	−838.705	−192.036	1.967
5200	63.754	393.329	336.172	297.219	−838.736	−179.357	1.802
5300	63.857	394.545	337.262	303.600	−838.777	−166.675	1.643
5400	63.961	395.739	338.333	309.991	−838.828	−153.994	1.490
5500	64.065	396.914	339.388	316.392	−838.889	−141.312	1.342
5600	64.169	398.069	340.425	322.804	−838.962	−128.627	1.200
5700	64.273	399.206	341.447	329.226	−839.048	−115.942	1.062
5800	64.377	400.324	342.452	335.658	−839.149	−103.254	0.930
5900	64.480	401.426	343.443	342.101	−839.266	−90.567	0.802
6000	64.582	402.510	344.418	348.554	−839.400	−77.875	0.678

PREVIOUS June 1968 (1 atm)   CURRENT. June 1968 (1 bar)

Boron Oxide, Ion (BO_2^-) IDEAL GAS $M_r = 42.80935$ Boron Oxide, Ion (BO_2^-) $B_1O_2^-(g)$

$S^\circ(298.15\ K) = [215.9 \pm 8.4]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH^\circ(0\ K) = -688 \pm 25\ kJ{\cdot}mol^{-1}$
$\Delta_fH^\circ(298.15\ K) = -695 \pm 25\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights State	ϵ_i, cm^{-1}	g_i
$^1\Sigma_g^+$	0	1
$^1B_2$	[35000]	1

Vibrational Frequencies and Degeneracies ν, cm^{-1}
[1150] (1)
[580] (2)
[2200] (1)

Point Group: $[D_{\infty h}]$ $\sigma = 2$
Bond Distance: B–O = [1.25] Å
Bond Angle: O–B–O = [180]°
Rotational Constant: $B_0 = [0.337159]\ cm^{-1}$

Enthalpy of Formation

Jensen[4] has obtained equilibrium constants for the reaction $HBO_2 + e^- \rightarrow H + BO_2^-$. This involves several assumptions the most basic of which is that boron added to $H_2/N_2/O_2$ flames is converted completely to HBO_2. The free electrons are produced by addition of potassium to the flame, and their concentration is measured directly by a microwave cavity resonance method. The hydrogen atom concentration is taken from previous studies on such flames. The BO_2^- concentration is obtained from the difference between the K^+ concentration and the free electron measurement. The K^+ concentration is measured by an electrostatic probe.

By 2nd and 3rd analysis of the data, 11 points read back from a plot, we obtain Δ_rH°(II, 298.15 K) = 27.5 ± 4 $kcal{\cdot}mol^{-1}$ and Δ_rH° (III, 298.15 K) = 20 ± 2 $kcal{\cdot}mol^{-1}$ with a drift of −3.7 ± 1.5 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$. The 3rd law value yields $\Delta_fH^\circ(BO_2^-$, 298 15 K) = −166 ± 6 $kcal{\cdot}mol^{-1}$ where the uncertainty includes possible errors in the functions. This corresponds to an electron affinity of BO_2 equal to 98 ± 6 $kcal{\cdot}mol^{-1}$ (4.25 eV).

Heat Capacity and Entropy

The molecular structure is assumed to be linear using the Walsh[1] prediction for 16 valence electron XY_2 molecules. The electronic states are taken from those for $CO_2(g)$ (2), which is isoelectronic with BO_2^- (g). The electronic level 35000 cm^{-1} and vibrational frequencies are estimated by comparison with the corresponding values for CO_2, CO_2^+, and BO_2, and, the data of Vasco and Srb[3] on the BO_2^- ion in alkali halide lattices. The B–O bond distance in $BO_2^-(g)$ is assumed to be smaller than the B–O bond in $BO_2(g)$, because the $BO_2^-(g)$ molecule has one more bonding electron than the $BO_2(g)$ molecule.

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0	0.	0.	INFINITE	−9.629	−688.078		
100	29.376	179.892	247.061	−6.717			
200	33.849	201.391	219.337	−3.589			
250	36.665	209.250	216.552	−1.826			
298.15	39.119	215.922	215.922	0.	−694.544	−689.762	120.843
300	39.207	216.164	215.923	0.072	−694.585	−689.733	120.093
350	41.425	222.378	216.408	2.090	−695.711	−688.835	102.803
400	43.352	228.039	217.514	4.210	−696.860	−687.774	89.814
450	45.040	233.244	218.976	6.421	−698.033	−686.569	79.695
500	46.533	238.069	220.647	8.711	−699.228	−685.231	71.586
600	49.058	246.784	224.293	13.495	−701.663	−682.204	59.391
700	51.105	254.506	228.068	18.507	−704.140	−678.765	50.650
800	52.779	261.443	231.813	23.704	−706.641	−674.970	44.071
900	54.151	267.741	235.461	29.052	−709.158	−670.860	38.936
1000	55.280	273.507	238.981	34.526	−711.687	−666.469	34.813
1100	56.213	278.821	242.365	40.102	−714.229	−661.824	31.427
1200	56.988	283.746	245.610	45.763	−716.784	−656.947	28.596
1300	57.635	288.334	248.722	51.495	−719.355	−651.857	26.192
1400	58.179	292.626	251.707	57.287	−721.945	−646.567	24.124
1500	58.638	296.656	254.570	63.128	−724.558	−641.092	22.325
1600	59.030	300.453	257.320	69.012	−727.196	−635.442	20.745
1700	59.365	304 042	259.964	74.932	−729.863	−629.626	19.346
1800	59.654	307.444	262.508	80.884	−732.561	−623.652	18.098
1900	59.904	310.676	264.959	86.862	−735.292	−617.527	16.977
2000	60.122	313.754	267.322	92.863	−738.059	−611.258	15.964
2100	60.314	316.692	269.604	98.885	−740.864	−604.849	15.045
2200	60.482	319.502	271.809	104 925	−743.707	−598.305	14.206
2300	60.631	322.194	273.941	110.981	−746.592	−591.632	13.436
2400	60.763	324.777	276.006	117.051	−799.777	−583.763	12.705
2500	60.881	327.260	278.007	123.133	−802.823	−574.700	12.008
2600	60.986	329.650	279.947	129.227	−805.879	−565.515	11.361
2700	61.081	331.953	281.831	135.330	−808.947	−556.211	10.761
2800	61.166	334.176	283 661	141.442	−812.026	−546.794	10.201
2900	61.243	336.324	285.440	147.563	−815.117	−537.268	9.677
3000	61.314	338.401	287.171	153 691	−818.219	−527.634	9.187
3100	61.377	340.413	288.856	159.825	−821.334	−517.896	8.726
3200	61.436	342.363	290.498	165.966	−824.461	−508.058	8.293
3300	61.489	344.254	292.099	172.112	−827.599	−498.123	7.885
3400	61.538	346.090	293.660	178.264	−830.749	−488.091	7.499
3500	61.583	347.875	295.183	184.420	−833.910	−477.967	7.133
3600	61.625	349.610	296.671	190.580	−837.083	−467.752	6.787
3700	61.663	351.299	298.125	196.745	−840.266	−457.450	6.458
3800	61.699	352.944	299.546	202.913	−843.460	−447.059	6.145
3900	61.733	354.547	300.936	209.085	−846.664	−436.586	5.847
4000	61.764	356.111	302.296	215.259	−849.878	−426.031	5.563
4100	61.794	357.636	303.627	221.437	−853.103	−415.395	5.292
4200	61.822	359.125	304.931	227.618	−1336.186	−397.656	4 946
4300	61.848	360.580	306.208	233.802	−1338.343	−375.284	4.559
4400	61.873	362.003	307.460	239.988	−1340.511	−352.863	4.189
4500	61.897	363.393	308.688	246.176	−1342.690	−330.392	3.835
4600	61.921	364.754	309.892	252.367	−1344.882	−307.873	3.496
4700	61.943	366.086	311.073	258.560	−1347.087	−285.305	3.171
4800	61.965	367.390	312.233	264.756	−1349.304	−262.690	2.859
4900	61.986	368.668	313.372	270.953	−1351.536	−240.029	2.559
5000	62.008	369.921	314.490	277.153	−1353.781	−217.322	2.270
5100	62.028	371.149	315.589	283.355	−1356.042	−194.570	1.993
5200	62.049	372.353	316.669	289.559	−1358.319	−171.775	1.726
5300	62.070	373.536	317.731	295.765	−1360.613	−148.934	1.468
5400	62.091	374.696	318.775	301.973	−1362.925	−126.051	1.219
5500	62.112	375.836	319.802	308.183	−1365.256	−103.125	0.979
5600	62.133	376.955	320.813	314.395	−1367.607	−80.155	0.748
5700	62.154	378.055	321.808	320.609	−1369.980	−57.144	0.524
5800	62.176	379.136	322.787	326.826	−1372.375	−34.091	0.307
5900	62.198	380.199	323.751	333.045	−1374.795	−10.998	0.097
6000	62.221	381.245	324.700	339.265	−1377.239	12.139	−0.106

PREVIOUS: December 1968 (1 atm) CURRENT: December 1968 (1 bar)

Boron Oxide, Ion (BO_2^-) $B_1O_2^-(g)$

$S°(298.15\ K) = 216.19 \pm 0.42\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 240.0 \pm 17\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 243.1 \pm 17.0\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$X^2\Sigma^+$	0	2
$A^2\Pi$	15663 15996	2
$B^2\Sigma^+$	35849	2
$C^2\Pi$	38782 38897	2

$\omega_e = 1188.14\ cm^{-1}$ $\omega_e x_e = 6.397\ cm^{-1}$ $\sigma = 1$
$B_e = 0.80586\ cm^{-1}$ $\alpha_e = 0.00617\ cm^{-1}$ $r_e = 1.609\ Å$

Enthalpy of Formation

Gingerich,[1] empolying mass spectrometric investigations of the Au–Ce–CeS–BN–C system from a tungsten Knudsen effusion cell, reports two values of the BS(g) dissociation energy. The reaction enthalplies were evaluated by the 3rd law method. The two values reported are 140.4 ± 6.0 kcal·mol^{-1}, based on the dissociation energy of CS(g), and 145.4 ± 6.0 kcal·mol^{-1}, based on the dissociation energy of CeS(g).

Uy and Drowart[2] also studied the dissociation energy of BS(g) by two different exchange reactions using mass spectrometric Knudsen cell techniques. Molybdenum cells were used. Based on an exchange between B(g) and YS(g), they reported $D_0° = 138.8 \pm 3.2$ kcal·mol^{-1} for BS(g). A second determination based on an exchange between BO(g) and YS(g) was reported as $D_0° = 137.0 \pm 3.2$ kcal·mol^{-1}

Gaydon[3] suggests a value of 118 kcal·mol^{-1} for the dissociation energy based on two linear Birge–Sponer extrapolations from the data of Zeeman.[4] This data gave values of 154.5 kcal·mol^{-1} and 131.4 kcal·mol^{-1} for extrapolations from the ground state and $A^2\Pi$ state, respectively. McDonald and Innes[5] extended Zeeman's analysis,[4] examined perturbative effects, and calculated $\omega_e y_e = -0.004\ cm^{-1}$ for the ground state. This perturbative interpretation was supported by Singh, Tewari, and Mohan.[7] Accounting for $\omega_e y_e$ value, the Birge–Sponer extrapolation yields a value $D_0° = 142.3$ kcal·mol^{-1} for BS(g). This value was adjusted to 140.0 kcal·mol^{-1} using an ionic character correction factor as suggested by Hildenbrand and Murad.[6]

The value of 140 0 ± 4.0 kcal·mol^{-1} for the dissociation energy of BS(g) is chosen as the best value. It is an average of the four reported thermochemical values and is the adjusted Birge–Sponer value, the adjustment arising from a correction technique which has been shown to be quite dependable. This value leads to a enthalpy of formation $\Delta_f H°(298.15\ K) = 58.1 \pm 4.0$ kcal·mol^{-1}.

Heat Capacity and Entropy

The spectroscopic constants for the $X^2\Sigma^+$ state are from Zeeman[4] and are corrected to account for the natural abundances of the elements. The electronic states X, A, and C are reported by Zeeman.[4] The $B^2\Sigma^+$ state is reported by McDonald and Innes.[5]

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	-8.724	239.992	239.992	INFINITE
100	29.106	184.196	242.369	-5.817	242.185	225.049	-117.553
200	29.239	204.389	218.907	-2.903	243.124	207.457	-54.182
250	29.557	210.944	216.682	-1.434	243.203	198.527	-41.480
298.15	30.051	216.190	216.190	0.	243.090	189.930	-33.275
300	30.073	216.376	216.191	0.056	243.083	189.600	-33.012
350	30.706	221.058	216.559	1.575	242.809	180.706	-26.969
400	31.376	225.202	217.385	3.127	240.195	171.948	-22.454
450	32.028	228.936	218.465	4.712	239.027	163.478	-18.976
500	32.631	232.342	219.685	6.329	237.738	155.155	-16.209
600	33.656	238.386	222.310	9.645	235.488	138.854	-12.088
700	34.449	243.636	224.990	13.052	233.393	122.915	-9.172
800	35.057	248.278	227.617	16.529	231.376	107.271	-7.004
900	35.527	252.435	230.147	20.059	176.267	92.958	-5.395
1000	35.895	256.198	232.567	23.631	175.521	83.741	-4.374
1100	36.188	259.634	234.874	27.236	174.724	74.601	-3.542
1200	36.426	262.793	237.071	30.867	173.879	65.536	-2.853
1300	36.622	265.716	239.163	34.519	172.988	56.543	-2.272
1400	36.786	268.437	241.158	38.190	172.051	47.620	-1.777
1500	36.926	270.979	243.062	41.876	171.069	38.766	-1.350
1600	37.046	273.367	244.882	45.575	170.043	29 979	-0.979
1700	37.153	275.616	246.625	49.285	168.974	21.258	-0.653
1800	37.249	277.742	248.295	53.005	167.864	12.601	-0.366
1900	37.338	279.758	249.898	56.734	166.712	4.006	-0.110
2000	37.421	281.676	251.440	60.472	165.521	-4.527	0.118
2100	37.502	283.504	252.923	64.218	164.292	-12.999	0.323
2200	37.583	285.250	254.353	67.973	163.027	-21.412	0.508
2300	37.664	286.922	255.733	71.735	161.727	-29.767	0.676
2400	37.749	288.527	257.066	75.506	110.133	-36.995	0.805
2500	37.838	290.070	258.356	79.285	108.689	-43.096	0.900
2600	37 933	291.556	259.604	83.073	107.246	-49.139	0.987
2700	38.033	292.989	260.815	86.872	105.808	-55.126	1.066
2800	38.142	294.374	261.989	90.680	104.373	-61.060	1.139
2900	38.257	295.715	263.129	94.500	102.945	-66.944	1.206
3000	38.381	297.014	264.236	98.332	101.523	-72.777	1.267
3100	38.513	298.274	265.314	102.177	100.109	-78.564	1.324
3200	38.653	299.499	266.363	106.035	98.705	-84.305	1.376
3300	38.801	300.691	267.386	109.908	97.310	-90.003	1.425
3400	38.957	301.852	268.382	113.795	95.927	-95.658	1.470
3500	39.120	302.983	269.355	117.699	94.555	-101.273	1.511
3600	39.289	304.088	270.304	121.620	93.196	-106.849	1.550
3700	39.466	305.167	271.232	125.557	91.850	-112.387	1.587
3800	39.647	306.221	272.139	129.513	90.518	-117.889	1.621
3900	39.834	307.254	273.026	133.487	89.200	-123.356	1.652
4000	40.026	308.265	273.895	137.480	87.897	-128.790	1.682
4100	40.221	309.255	274.745	141.492	86.607	-134.191	1.710
4200	40.419	310.227	275.578	145.524	-394.516	-132.537	1.648
4300	40.620	311.180	276.395	149.576	-394.688	-126.297	1.534
4400	40.822	312.117	277.197	153.648	-394.847	-120.054	1.425
4500	41.026	313.036	277.983	157.741	-394.994	-113.807	1.321
4600	41.230	313.940	278.755	161.853	-395.128	-107.557	1.221
4700	41.435	314.829	279.513	165.987	-395.250	-101.304	1.126
4800	41.639	315.704	280.258	170.140	-395.360	-95.048	1.034
4900	41.842	316.564	280.990	174.314	-395.460	-88.791	0.947
5000	42.043	317.412	281.710	178.509	-395.549	-82.531	0.862
5100	42.243	318.246	282.418	182.723	-395.629	-76.270	0.781
5200	42.441	319.068	283.115	186.957	-395.700	-70.008	0.703
5300	42.637	319.879	283.801	191.211	-395.763	-63.744	0.628
5400	42.830	320.677	284.477	195.484	-395.818	-57.479	0.556
5500	43.019	321.465	285.142	199.777	-395.866	-51.213	0.486
5600	43.206	322.242	285.797	204.088	-395.908	-44.946	0.419
5700	43.390	323.008	286.444	208.418	-395.945	-38.678	0.354
5800	43.569	323.764	287.081	212.766	-395.978	-32.410	0.292
5900	43.746	324.511	287.709	217.132	-396.007	-26.142	0.231
6000	43.918	325.247	288.328	221.515	-396.032	-19.872	0.173

PREVIOUS. June 1972 (1 atm) CURRENT: June 1972 (1 bar)

Titanium Boride (TiB) CRYSTAL $M_r = 58.69$ Titanium Boride (TiB) $B_1Ti_1(cr)$

$\Delta_fH°(0\ K)$ = Unknown

$S°(298.15\ K) = [34.7 \pm 6.3]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298.15\ K) = -160.2 \pm 38\ kJ{\cdot}mol^{-1}$

$T_{dcm} = [2500]\ K$

Entholpy of Formation

Schissel and Trulson[1] used a mass spectrometer with Knudsen cells to study the vaporization of the titanium–boron system and obtained $\Delta_rG°(2340\ K) = -118.54\ kcal{\cdot}mol^{-1}$ for the reaction TiB(c) = Ti(g) + B(g). This corresponds to $\Delta_fG°(TiB,\ cr,\ 2340\ K) = -33.266 \pm 9\ kcal{\cdot}mol^{-1}$, where $4\ kcal{\cdot}mol^{-1}$ of the uncertainty is due to the enthalpy of sublimation of boron. When this is reduced to 298 15 K one obtains $\Delta_fH°(TiB,\ cr,\ 298.15\ K) = -38.3 \pm 9\ kcal{\cdot}mol^{-1}$. This value implies a high stability for TiB. This is also indicated by the phase studies of Nowotny *et al.*[2]

Heat Capacity and Entropy

The heat capacities fron 298 to 1200 K were estimated from that of TiB_2 by assuming the difference to be the same as that between CrB and CrB_2 as determined by R. Mezaki, E. W. Tilleux, D. W. Barnes and J. L. Margrave (Paper presented at the International Symposium on Nuclear Materials, Vienna, May 1962). A linear extrapolation was assumed above 1200 K.

The heat capacities above 298 K were also estimated from the relationship $C_p(Ti) + C_p(2B) - C_p(TiB_2) = 2/3\ [C_p(Ti) + C_p(B) - C_p(TiB)]$. This estimation agreed with the above to 4% over the temperature range 400 to 1000 K.

$S°(TiB,\ cr,\ 298.15\ K) = 8.3\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ was calculated by the method of Latimer.[3] Using JANAF $S°(TiB_2,\ cr,\ 298.15\ K) = 6.8\ cal^{-1}\ K^{-1}{\cdot}mol^{-1}$ and Latimer's value of $9.8\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ for the entropy contribution of Ti, an entropy contribution of $-1.5\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ per boron atom was calculated.

Decomposition Data

The phase diagram given by McQuillan and McQuillan[4] was used to estimate the decomposition temperature. This diagram shows the decomposition products are TiB_2 and Ti_2B. However, Nowotny *et al.*[2] have shown Ti_2B to be nonexistent and so the decomposition products are not defined; probably an eutectic of TiB and TiB_2 is involved.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200							
250							
298.15	29.673	34.727	34.727	0.	−160.247	−159.691	27.977
300	29.916	34.911	34.728	0.055	−160.260	−159.687	27.804
400	40.334	45.065	36.041	3.610	−160.681	−159.420	20.818
500	45.714	54 690	38.824	7.933	−160.829	−159.085	16.620
600	48.568	63.297	42.200	12.658	−160.911	−158.729	13.819
700	50.124	70.910	45.769	17.599	−161.013	−158.358	11.817
800	50.911	77.657	49.341	22.652	−161.167	−157.968	10.314
900	51.488	83.688	52.829	27.774	−161.419	−157.555	9.144
1000	51.915	89.137	56.191	32.945	−161.831	−157.105	8.206
1100	52.191	94.099	59.415	38.152	−162.469	−156.604	7.436
1200	52.325	98.646	62.498	43.377	−167.327	−155.914	6.787
1300	52.459	102.839	65.442	48.617	−167.710	−154.948	6.226
1400	52.593	106.732	68.254	53.869	−168.206	−153.948	5.744
1500	52.727	110.365	70.941	59.135	−168.824	−152.909	5.325
1600	52.861	113.772	73.513	64.415	−169.576	−151.824	4.957
1700	52.995	116.981	75.976	69.707	−170.472	−150.688	4.630
1800	53.128	120.014	78.339	75.013	−171.524	−149.495	4.338
1900	53.262	122.890	80.609	80.333	−172.744	−148.239	4.075
2000	53.396	125.625	82.792	85.666	−188.831	−146.460	3.825
2100	53.530	128.233	84.894	91.012	−191.171	−144.284	3.589
2200	53.664	130.727	86.921	96.372	−193.532	−141.996	3.371
2300	53.798	133.115	88.878	101.745	−195.913	−139.600	3.170
2400	53.932	135.408	90.770	107.132	−248.574	−136.032	2.961
2500	54.066	137.612	92.599	112.531	−251.073	−131.291	2.743
2600	54.200	139.735	94.372	117.945	−253.558	−126.451	2.540
2700	54.333	141.783	96.090	123.371	−256.030	−121.515	2.351
2800	54.467	143.762	97.757	128.811	−258.489	−116.488	2.173
2900	54.601	145.675	99.377	134.265	−260.934	−111.373	2.006
3000	54.735	147.528	100.951	139.732	−263.366	−106.174	1.849
3100	54.869	149.325	102.483	145.212	−265.785	−100.895	1.700
3200	55.003	151.070	103.974	150.705	−268.190	−95.537	1.559
3300	55.137	152.764	105.427	156.212	−270.582	−90.105	1.426
3400	55.271	154.412	106.844	161.733	−272.960	−84.600	1.300
3500	55.405	156.016	108.226	167.267	−275.325	−79.026	1.179
3600	55.538	157.579	109.575	172.814	−277.677	−73.384	1.065
3700	55.672	159.102	110.893	178.374	−689.113	−59.888	0.845
3800	55.806	160.589	112.181	183.948	−690.204	−42.868	0.589
3900	55.940	162.040	113.441	189.535	−691.336	−25.818	0.346
4000	56.074	163.458	114.674	195.136	−692.509	−8.739	0.114

PREVIOUS. March 1963 CURRENT: June 1965

$S°(298.15\ K) = 202.07 \pm 0.17\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 823.3 \pm 33.5\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 829.7 \pm 33.5\ kJ{\cdot}mol^{-1}$

Electronic and Molecular Constants ($\sigma = 2$)

State	ϵ_i, cm^{-1}	g_i	ω_e, cm^{-1}	$\omega_e x_e$, cm^{-1}	B_e, cm^{-1}	α_e, cm^{-1}	r_e, Å	Source
$^3\Sigma_g^-$	0.0	3	1061.61	9.536	1.236121	0.01442411	1.589	1,2,3
$^5\Sigma_u^-$	[1271.]	[5]	[1215.81]	[9.995]	[1.305]	[0.0113]	[1.546]	4
$1^3\Sigma_u^-$	[14829.]	[3]	[1114.83]	[16.318]	[1.275]	[0.0175]	[1.565]	4
$2^3\Sigma_u^-$	30573.4	3	946.59	2.652	1.183086	0.01133323	1.625	1,2,3

Enthalpy of Formation

The equilbrium vapor pressure of the reaction $B_2(g) \rightarrow B(g) + B(cr)$ was determined by Verhaegen and Drowart.[5] Using the value, $p(B_2,g)/p(B,g) = 9 \times 10^{-5}$ at 2330 K where p is partial pressure, the enthalpy of reaction, $\Delta_r H°(298.15\ K)$, was evaluated by the 3rd law method to be $-64.5 \pm 5.0\ kcal{\cdot}mol^{-1}$. Using auxiliary data,[6] this leads to $\Delta_f H°(298.15\ K) = 198.3 \pm 8.0\ kcal{\cdot}mol^{-1}$ for $B_2(g)$ or $D_0^\circ = 2.97 \pm 0.61$ eV.

Heat Capacity and Entropy

The thermodynamic functions are calculated using first order anharmonic corrections to Q_r^i and Q_v^i in the partition function $Q = Q_t \Sigma Q_r^i Q_v^i g_i \exp(-c_2\epsilon_i/T)$. Molecular and spectroscopic constants for the $^3\Sigma_g^-$ ground state and the $2^3\Sigma_u^-$ state are taken from a study[3] which revises the values of Douglas and Herzberg.[1 2] The molecular constants and electronic levels for the lowest $^5\Sigma_u^-$ state and $1^3\Sigma_u^-$ state are based on the ab initio configuration interaction calculations of Dupuis and Liu.[4] These calculations, along with the optical absorption and ESR spectra of B_2 at 4 K reported by Graham and Weltner,[7] support a $^3\Sigma_g^-$ ground state rather than $^5\Sigma_u^-$ favored by previous ab initio work.[8 9] All molecular and spectroscopic constants have been corrected to the average isotopic species.

Differences between our calculated thermodynamic functions and those given by Feber and Herrick[10] *using direct summation techniques* can be attributed to inclusion of the low lying $^5\Sigma_u^-$ state and $1^3\Sigma_u^-$ state in our calculations. The JANAF adopted entropy is 0.35–1.6 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ higher than their values in the 500–600 K temperature range. The JANAF adopted heat capacities are also higher in the low temperature range, 0.2–0.9 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ larger between 298–1000 K. A comparison of the thermodynamic functions calculated using only *the ground and upper* $2^3\Sigma_u^-$ *state shows no major* numerical difference with this earlier tabulation,[10] however.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8.810	823.305	823.305	INFINITE
100	29.111	169.727	228.775	−5.905	826.162	809.251	−422.709
200	29.500	189.962	204.880	−2.984	828.418	791.393	−206.691
250	30.345	196.626	202.585	−1.490	829.169	782.044	−163.399
298.15	31.594	202.072	202.072	0.	829.687	772.918	−135.412
300	31.648	202.268	202.073	0.058	829.704	772.566	−134.516
350	33.187	207.260	202.464	1.679	830.070	763.012	−113.873
400	34.737	211.794	203.351	3.377	830.297	753.415	−98.386
450	36.146	215.969	204.524	5.150	830.415	743.797	−86.338
500	37.335	219.841	205.864	6.988	830.446	734.170	−76.698
600	39.012	226.809	208.788	10.813	830.309	714.924	−62.240
700	39.916	232.899	211.807	14.765	829.950	695.719	−51.915
800	40.310	238.259	214.785	18.779	829.399	676.578	−44.176
900	40.410	243.015	217.663	22.817	828.673	657.517	−38.161
1000	40.355	247.271	220.415	26.856	827.788	638.546	−33.354
1100	40.226	251.111	223.033	30.886	826.758	619.671	−29.426
1200	40.071	254.605	225.521	34.901	825.595	600.895	−26.156
1300	39.914	257.806	227.883	38.900	824.311	582.221	−23.394
1400	39.766	260.758	230.127	42.884	822.915	563.651	−21.030
1500	39.632	263.497	232.262	46.853	821.417	545.183	−18.985
1600	39.516	266.051	234.295	50.811	819.821	526.819	−17.199
1700	39.416	268.444	236.234	54.757	818.135	508.558	−15.626
1800	39.332	270.694	238.086	58.694	816.363	490.398	−14.231
1900	39.263	272.819	239.859	62.624	814.510	472.339	−12.986
2000	39.207	274.832	241.558	66.547	812.578	454.380	−11.867
2100	39.164	276.743	243.188	70.466	810.572	436.519	−10.858
2200	39.132	278.564	244.755	74.381	808.492	418.755	−9.943
2300	39.110	280.303	246.263	78.293	806.343	401.088	−9.109
2400	39.098	281.968	247.716	82.203	703.606	385.653	−8.394
2500	39.095	283.564	249.119	86.112	701.166	372.455	−7.782
2600	39.099	285.097	250.473	90.022	698.725	359.355	−7.220
2700	39.112	286.573	251.783	93.933	696.286	346.349	−6.701
2800	39.131	287.996	253.051	97.845	693.848	333.432	−6.220
2900	39.156	289.369	254.280	101.759	691.412	320.603	−5.775
3000	39.188	290.697	255.472	105.676	688.979	307.858	−5.360
3100	39.224	291.983	256.629	109.597	686.550	295.195	−4.974
3200	39.266	293.229	257 753	113.521	684.124	282.609	−4.613
3300	39.312	294.438	258.847	117.450	681.703	270.099	−4.275
3400	39.362	295.612	259.911	121.384	679.287	257.662	−3.958
3500	39.416	296.754	260.947	125.323	676.876	245.297	−3.661
3600	39.474	297.865	261.957	129.267	674.470	233.000	−3.381
3700	39.534	298.947	262.943	133.217	672.071	220.770	−3.117
3800	39.597	300.002	263.904	137.174	669.677	208.605	−2.867
3900	39.663	301.032	264.843	141.137	667.290	196.502	−2.632
4000	39.731	302.037	265.760	145.107	664.910	184.461	−2.409
4100	39.801	303.019	266.657	149.083	662.536	172.479	−2.197
4200	39.872	303.979	267.534	153.067	−299.529	174.604	−2.172
4300	39.945	304.918	268.393	157.058	−299.713	185.895	−2.258
4400	40.020	305.837	269.233	161.056	−299.894	197.190	−2.341
4500	40.095	306.737	270.057	165.062	−300.072	208.489	−2.420
4600	40.172	307.619	270.864	169.075	−300.247	219.793	−2.496
4700	40.249	308.484	271.655	173.096	−300.418	231.100	−2.568
4800	40.328	309.332	272.431	177.125	−300.588	242.411	−2.638
4900	40.406	310.164	273.193	181.162	−300.757	253.725	−2.705
5000	40.486	310.982	273.940	185.206	−300.924	265.042	−2.769
5100	40.565	311.784	274.675	189.259	−301.091	276.363	−2.831
5200	40.645	312.573	275.396	193.319	−301.258	287.688	−2.890
5300	40.725	313.348	276.105	197.388	−301.426	299.015	−2.947
5400	40.805	314.110	276.801	201.464	−301.596	310.346	−3.002
5500	40.885	314.859	277.487	205.549	−301.768	321.680	−3.055
5600	40.966	315.596	278.160	209.641	−301.942	333.017	−3.106
5700	41.046	316.322	278.824	213.742	−302.121	344.357	−3.156
5800	41 126	317.037	279.476	217.850	−302.303	355.700	−3.203
5900	41.206	317.740	280.119	221.967	−302.491	367.046	−3.250
6000	41.285	318.434	280.752	226.092	−302.685	378.396	−3.294

PREVIOUS: March 1979 (1 atm) CURRENT: March 1979 (1 bar)

Beryllium Borate ($Be(BO_2)_2$) IDEAL GAS $M_r = 94.62978$ Beryllium Borate ($Be(BO_2)_2$) $B_2Be_1O_4(g)$

$S°(298.15\ K) = [326.79]\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = -1348 \pm 42\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = -1351 \pm 42\ kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
[2000](1)	[1050](1)	[400](1)
[1600](1)	[650](1)	[350](1)
[1200](1)	[650](1)	[200](1)
[1200](1)	[600](1)	[150](1)
[1050](1)	[500](1)	[120](1)

Ground State Quantum Weight: [1] $\sigma = 2$
Point Point: [C_{2h}]
Bond Distances: Be–O = [1.63] Å; O–B = [1.34] Å; B=O = [1.20] Å
Bond Angles: O=B–O = [180]°; O–Be–O = [180]°; B–O–Be = [95]°
Product of the Moments of Inertia: $I_AI_BI_C = [5.382534 \times 10^{-113}]\ g^3·cm^6$

Enthalpy of Formation

The enthalpy of formation was obtained from mass spectrometric studies; the following reactions at 1500 K were reported by Blackburn and Buchler.[1]

Reaction	$\Delta_r H°$, kcal·mol^{-1}
1. $B_2O_3(l) \rightarrow B_2O_3(g)$	$\Delta H_1 = 92.226$
2. 1/3 $Be_3B_2O_6(cr)$ + 2/3 $B_2O_3(l) \rightarrow Be(BO_2)_2(g)$	$\Delta H_2 = 118 \pm 2$
3. $Be_3B_2O_6(cr) \rightarrow 3\ BeO(cr) + B_2O_3(g)$	$\Delta H_3 = 112 \pm 1$
4. $Be_3B_2O_6(cr) \rightarrow 2\ BeO(cr) + Be(BO_2)_2(g)$	$\Delta H_4 = 137 \pm 3$
5. $3\ BeO(cr) + B_2O_3(l) \rightarrow Be_3B_2O_6(cr)$	$\Delta H_5 = 23$
6. $BeO(cr) + B_2O_3(g) \rightarrow Be(BO_2)_2(g)$	$\Delta H_6 = 22$

ΔH_1 was obtained from JANAF values[2] for $B_2O_3(l)$ and $B_2O_3(g)$. The values for ΔH_2, ΔH_3, and ΔH_4 were obtained from Blackburn and Buchler.[1] ΔH_5 was obtained by taking the average of $\Delta H_5 = -20$ kcal·mol^{-1} in a weight loss experiment, $\Delta H_5 = \Delta H_1 - \Delta H_3 = -19.774$ kcal·mol^{-1}, and $\Delta H_5 = 3/2\ (\Delta H_2 - \Delta H_4) = 28.5$ kcal·mol^{-1}. The ΔH_6 value was obtained by taking the average of $\Delta H_6 = \Delta H_4 - \Delta H_3 = 25$ kcal·mol^{-1} and $\Delta H_6 = \Delta H_2 - \Delta H_1 + 1/3\ \Delta H_5 = 18.107$ kcal·mol^{-1}. The $\Delta_f H°(298.15\ K)$ of BeB_2O_4 was calculated from reaction 6 with auxiliary JANAF values.

Heat Capacity and Entropy

The vibrational frequencies estimated by comparison with B_2O_3 were adjusted to obtain an $S°(1500\ K) = 127$ obtained in a manner analogous with $\Delta_f H°$ from the report of Blackburn and Buchler.[1] The frequencies listed are not in point group order. All other molecular constants were estimated by comparison with related boron oxide molecules. The principal moments of inertia are $I_A = 8.5573 \times 10^{-39}$, $I_B = 75.1462 \times 10^{-39}$, and $I_C = 83.7035 \times 10^{-39}\ g·cm^2$.

References

[1] P. E. Blackburn and A. Buchler, Tech. Report No. 1 (1965).
[2] JANAF Thermochemical Tables: $B_2O_3(l)$ and $B_2O_3(g)$, 6–30–71.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
0	0.	0.	INFINITE	−18.639	−1348.345	−1348.345	INFINITE
100	52.679	250.301	396.063	−14.576	−1350.178	−1340.435	700.171
200	74.445	293.699	334.648	−8.190	−1350.857	−1330.401	347.465
250	83.774	311.333	328.252	−4.230	−1351.147	−1325.253	276.897
298.15	91.764	326.785	326.785	0.	−1351.432	−1320.240	231.301
300	92.053	327.354	326.787	0.170	−1351.443	−1320.047	229.841
350	99.380	342.106	327.935	4.960	−1351.739	−1314.791	196.222
400	105.839	355.807	330.573	10.094	−1352.029	−1309.492	171.002
450	111.510	368.608	334.096	15.530	−1352.309	−1304.158	151.383
500	116.475	380.619	338.154	21.233	−1352.572	−1298.794	135.684
600	124.603	402.607	347.099	33.305	−1353.048	−1287.993	112.130
700	130.814	422.303	356.460	46.090	−1353.475	−1277.116	95.300
800	135.589	440.096	365.821	59.420	−1353.880	−1266.180	82.673
900	139.296	456.289	374.987	73.172	−1354.296	−1255.193	72.849
1000	142.208	471.122	383.869	87.253	−1354.746	−1244.158	64.988
1100	144.522	484.788	392.430	101.594	−1355.254	−1233.074	58.554
1200	146.384	497.446	400.661	116.142	−1355.839	−1221.942	53.190
1300	147.899	509.225	408.564	130.859	−1356.517	−1210.757	48.649
1400	149.144	520.233	416.152	145.713	−1357.302	−1199.516	44.754
1500	150.179	530.559	423.438	160.681	−1358.206	−1188.215	41.377
1600	151.047	540.280	430.440	175.743	−1373.776	−1176.324	38.403
1700	151.781	549.459	437.174	190.886	−1374.547	−1163.960	35.764
1800	152.406	558.153	443.655	206.096	−1375.398	−1151.549	33.417
1900	152.943	566.408	449.901	221.364	−1376.333	−1139.087	31.316
2000	153.407	574.265	455.924	236.682	−1377.357	−1126.575	29.423
2100	153.811	581.760	461.739	252.043	−1378.476	−1114.008	27.709
2200	154.164	588.923	467.359	267.443	−1379.693	−1101.385	26.150
2300	154.475	595.783	472.794	282.875	−1381.011	−1088.707	24.725
2400	154.750	602.364	478.057	298.336	−1482.951	−1073.831	23.371
2500	154.994	608.686	483.156	313.824	−1484.633	−1056.750	22.080
2600	155.211	614.769	488.102	329.334	−1486.357	−1039.600	20.886
2700	155.406	620.631	492.903	344.865	−1488.124	−1022.383	19.779
2800	155.581	626.286	497.566	360.415	−1780.891	−998.878	18.634
2900	155.739	631.748	502.099	375.981	−1781.683	−970.936	17.488
3000	155.882	637.030	506.509	391.562	−1782.504	−942.965	16.418
3100	156.012	642.144	510.803	407.157	−1783.354	−914.965	15.417
3200	156.130	647.099	514.985	422.764	−1784.236	−886.940	14.478
3300	156.237	651.905	519.062	438.382	−1785.150	−858.886	13.595
3400	156.336	656.570	523.038	454.011	−1786.098	−830.802	12.764
3500	156.427	661.103	526.918	469.649	−1787.082	−802.692	11.980
3600	156.510	665.511	530.707	485.296	−1788.103	−774.552	11.238
3700	156.587	669.801	534.408	500.951	−1789.161	−746.384	10.537
3800	156.658	673.977	538.027	516.613	−1790.260	−718.184	9.872
3900	156.723	678.048	541.565	532.283	−1791.400	−689.957	9.241
4000	156.784	682.016	545.027	547.958	−1792.584	−661.701	8.641
4100	156.841	685.888	548.415	563.639	−1793.812	−633.413	8.070
4200	156.893	689 668	551.734	579.326	−2754.787	−591.047	7.351
4300	156.942	693.361	554.985	595.018	−2753.937	−539.539	6.554
4400	156.988	696.969	558.171	610.714	−2753.143	−488.052	5.794
4500	157.031	700.498	561.294	626.415	−2752.406	−436.582	5.068
4600	157.071	703.950	564.358	642.121	−2751.729	−385.127	4.373
4700	157.109	707.328	567.364	657.830	−2751.115	−333.685	3.708
4800	157.144	710.636	570.315	673.542	−2750.568	−282.256	3.072
4900	157.177	713.877	573.212	689.258	−2750.089	−230.837	2.461
5000	157.209	717.052	576.057	704.978	−2749.682	−179.428	1.874
5100	157.238	720.166	578.852	720.700	−2749.350	−128.026	1.311
5200	157.266	723.219	581.599	736.425	−2749.096	−76.632	0.770
5300	157.292	726.215	584.300	752.153	−2748.923	−25.238	0.249
5400	157.317	729.156	586.955	767.884	−2748.834	26.150	−0.253
5500	157.340	732.042	589.567	783.616	−2748.832	77.537	−0.736
5600	157.363	734.878	592.136	799.352	−2748.920	128.928	−1.203
5700	157.384	737.663	594.665	815.089	−2749.101	180.319	−1.652
5800	157.404	740.401	597.154	830.828	−2749.378	231.716	−2.087
5900	157.423	743.091	599.605	846.570	−2749.754	283.114	−2.507
6000	157.441	745.737	602.019	862.313	−2750.233	334.525	−2.912

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

Beryllium Borate ($Be_3B_2O_6$) CRYSTAL $M_r = 144.65294$ Beryllium Borate ($Be_3B_2O_6$) $B_2Be_3O_6(cr)$

$S°(298.15\ K) = [100 \pm 13]\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{fus} = 1768 \pm 5\ K$

$\Delta_f H°(0\ K) = $ Unknown
$\Delta_f H°(298.15\ K) = -3104 \pm 8\ kJ \cdot mol^{-1}$
$\Delta_{fus} H° = $ Unknown

Enthalpy of Formation

The adopted $\Delta_f H°(298.15\ K) = -741.96 \pm 2\ kcal \cdot mol^{-1}$ was calculated from $\Delta_r H°(298.15\ K) = -13.38 \pm 0.5\ kcal \cdot mol^{-1}$ for $3BeO(cr) + B_2O_3(g, l) = Be_3B_2O_6(cr)$ measured calorimetrically by Gross.[1] From equilibrium data relating to the same reaction at 1500 K, Blackburn and Buchler[2] report enthalpies of reaction of -21 ± 2 and $-28.5 \pm 5\ kcal \cdot mol^{-1}$ which correspond to -21.7 and $-29.2\ kcal \cdot mol^{-1}$ at 298.15 K. The discrepancy of 8 to 16 $kcal \cdot mol^{-1}$ is attributed primarily to the equilibrium values. These values result from differences between 2nd law enthalpies of reaction derived from the variation with temperature of ion intensities for $B_2O_3^+$ and $Be(BO_2)_2^+$, respectively, over the systems $B_2O_3(l)$–$Be_3B_2O_6(cr)$ and $Be_3B_2O_6(cr)$–$BeO(cr)$. The reported reactions and their heats are:

Reaction	$\Delta_r H°(1500\ K)$ $kcal \cdot mol^{-1}$
(a) $B_2O_3(l) \rightarrow B_2O_3(g)$	91 ± 0.5
(b) $Be_3B_2O_6(cr) \rightarrow 3\ BeO(cr) + B_2O_3(g)$	112 ± 1
(c) $1/3\ Be_3B_2O_6(cr) + 2/3\ B_2O_3(l) \rightarrow Be(BO_2)(g)$	118 ± 2
(d) $Be_3B_2O_6(cr) \rightarrow 2\ BeO(cr) + Be(BO_2)_2(g)$	137 ± 3

Heat Capacity and Entropy

The heat capacity was estimated from that for BeO(cr) and $B_2O_3(cr)$. The adopted $S°(298.15\ K) = 24 \pm 3$ eu is an average value from the following three estimates. Blackburn and Buchler[2] report $K_p = 2.7 \times 10^{-5}$ atm and 9.3×10^{-6} atm at 1500 K for reactions a and b (see enthalpy of formation), based on vacuum balance data and ion intensities, respectively. Three K_p's yield $\Delta_r G°(1500\ K) = -3.17\ kcal \cdot mol^{-1}$ for $3\ BeO(cr) + B_2O_3(l) \rightarrow Be_3B_2O_6(cr)$. Combining this with the JANAF value for $\Delta_r H°(1500\ K) = -12.64\ kcal \cdot mol^{-1}$, we get $\Delta_r S°(1500\ K) = -6.3$ and $S°(Be_3B_2O_6, cr, 298.15\ K) = 22.9\ cal \cdot K^{-1} \cdot mol^{-1}$. This entropy agrees with 23 $cal \cdot K^{-1} \cdot mol^{-1}$ estimated from the sum of entropies for the component oxides; however, the entropy for $Ca_3B_2O_6(cr)$ observed by Kelley *et al.*[3] is larger than that of the component oxides by 2.5 $cal \cdot K^{-1} \cdot mol^{-1}$. Use of this increment leads to 25.5 $cal \cdot K^{-1} \cdot mol^{-1}$ for $Be_3B_2O_6(cr)$.

Fusion Data

T_{fus} was obtained from Blackburn and Buchler.[2]

References

[1] P. Gross, Fulmer Research Institute, Report No. 5 (1966).
[2] P. E. Blackburn and A. Buchler, J. Phys. Chem. 69, 4250 (1965).
[3] K. K. Kelley, S. S. Todd and C. H. Shomate, J. Am. Chem. Soc. 70, 1350 (1948).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	139.746	100.416	100.416	0.	−3104.361	−2938.883	514.880
300	140.415	101.282	100.419	0.259	−3104.398	−2937.857	511.526
400	175.017	146.578	106.360	16.087	−3105.734	−2882.104	376.364
500	202.840	188.696	118.669	35.014	−3105.754	−2826.167	295.248
600	226.605	227.822	133.639	56.510	−3104.501	−2770.347	241.180
700	247.567	264.375	149.733	80.249	−3102.009	−2714.835	202.583
800	264.805	298.608	166.227	105.905	−3098.420	−2659.758	173.664
900	277.567	330.574	182.733	133.058	−3094.025	−2605.183	151.201
1000	286.269	360.294	199.021	161.272	−3089.170	−2551.124	133.257
1100	292.211	387.871	214.951	190.211	−3084.132	−2497.562	118.599
1200	296.395	413.483	230.442	219.650	−3079.092	−2444.461	106.405
1300	299.574	437.336	245.450	249.453	−3074.156	−2391.776	96.103
1400	302.210	459.635	259.961	279.544	−3069.382	−2339.466	87.287
1500	304.553	480.567	273.977	309.884	−3064.796	−2287.491	79.658
1600	306.729	500.292	287.512	340.448	−3104.023	−2234.237	72.940
1700	308.905	518.951	300.582	371.229	−3098.644	−2180.040	66.984
1800	311.206	536.674	313.210	402.235	−3093.254	−2126.161	61.700
1900	313.382	553.558	325.419	433.465	−3087.848	−2072.581	56.979
2000	315.474	569.686	337.232	464.907	−3082.437	−2019.285	52.738
2100	317.649	585.131	348.672	496.565	−3077.013	−1966.261	48.908
2200	319.658	599.955	359.759	528.431	−3071.583	−1913.494	45.432
2300	321.582	614.207	370.514	560.494	−3066.155	−1860.976	42.264
2400	323.423	627.932	380.956	592.745	−3161.256	−1806.557	39.319
2500	325.180	641.170	391.101	625.173	−3156.012	−1750.218	36.569
2600	327.105	653.962	400.966	657.789	−3150.710	−1694.091	34.035
2700	328.904	666.340	410.567	690.588	−3145.352	−1638.168	31.692
2800	330.829	678.337	419.917	723.575	−4012.804	−1563.777	29.173
2900	332.754	689.979	429.030	756.754	−4004.125	−1476.466	26.594
3000	334.720	701.293	437.918	790.127	−3995.326	−1389.454	24.193

PREVIOUS: CURRENT: September 1966

Dichloroborane ((BCl$_2$)$_2$) IDEAL GAS M_r = 163.432 Dichloroborane ((BCl$_2$)$_2$) B$_2$Cl$_4$(g)

$S°(298.15\ \mathrm{K}) = 358.96\ \mathrm{J{\cdot}K^{-1}{\cdot}mol^{-1}}$

$\Delta_f H°(0\ \mathrm{K})$ = Unknown
$\Delta_f H°(298.15\ \mathrm{K}) = -489.1 \pm 5.0\ \mathrm{kJ{\cdot}mol^{-1}}$

Vibrational Frequencies and Degeneracies		
υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}
1131(1)	Rotation	917(2)
401(1)	730(1)	617(2)
225(1)	291(1)	180(2)

Ground State Quantum Weight: 1 $\sigma = 4$
Point Group: D$_{2d}$
Bond Distances: B–Cl = 1.73 ± 0.02 Å; B–B = 1.75 ± 0.01 Å
Bond Angles: Cl–B–Cl = 120 ± 2°
Dihedral angle between two BCl$_2$ planes = 90°
Product of the Moments of Inertia: $I_A I_B I_C = 5.336257 \times 10^{-112}\ \mathrm{g^3{\cdot}cm^6}$

Enthalpy of Formation

Gunn *et al.*[1] determined the enthalpy change ($\Delta_r H°$) of the reaction $B_2Cl_4(l) + Cl_2(g) = 2\ BCl_3(g)$. From the value, $\Delta_r H°(298.15\ \mathrm{K}) = 67.3 \pm 0.6\ \mathrm{kcal{\cdot}mol^{-1}}$, the enthalpy of formation for B$_2$Cl$_4$(l) was calculated as $125.32 \pm 1.20\ \mathrm{kcal{\cdot}mol^{-1}}$. Based on $\Delta_{vap} H°(338.7\ \mathrm{K}) = 8.029\ \mathrm{kcal{\cdot}mol^{-1}}$ reported by Urry *et al.*,[2] the enthalpy of formation for B$_2$Cl$_4$(g) was derived to be $116.9 \pm 1.2\ \mathrm{kcal{\cdot}mol^{-1}}$.

Heat Capacity and Entropy

The vibrational frequencies, molecular structure and constants were taken from Mann and Fano.[3] The barrier restricting internal rotation about the B–B single bond is fixed at $1.53 \pm 0.60\ \mathrm{kcal{\cdot}mol^{-1}}$ obtained from Mason and Kreevoy.[4] The reduced moment of inertia for BCl$_2$ top is $I_r = 13.2149 \times 10^{-39}\ \mathrm{g{\cdot}cm^2}$. The principal moments of inertia are: $I_A = 52.8594 \times 10^{-39}$, $I_B = I_C = 100.4748 \times 10^{-39}\ \mathrm{g{\cdot}cm^2}$.

References

[1] S. R. Gunn, L. G. Green, and A. I. Von Egidy, J. Phys. Chem. 63, 1787 (1959).
[2] G. Urry, L. Wartik, R. E. Moore and H. I. Schlesinger, J. Am. Chem. Soc. 76, 5293 (1954).
[3] D. E. Mann and L. Fano, J. Chem. Phys. 26, 1665 (1957).
[4] E. A. Mason and M. M. Kreevoy, J. Am. Chem. Soc. 77, 5808 (1955).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0							
100	59.208	275.789	433.035	−15.725	−489.916	−479.632	250.534
200	80.655	323.936	367.210	−8.655	−489.588	−469.422	122.600
298.15	94.839	358.956	358.956	0.	−489.110	−459.631	80.526
300	95.056	359.543	358.958	0.176	−489.102	−459.448	79.997
400	104.801	388.301	362.812	10.195	−488.747	−449.622	58.715
500	111.307	412.425	370.388	21.019	−488.528	−439.868	45.953
600	115.683	433.124	379.160	32.378	−488.395	−430.149	37.448
700	118.541	451.179	388.187	44.095	−488.333	−420.448	31.374
800	120.792	467.162	397.079	56.066	−488.326	−410.751	26.819
900	122.242	481.475	405.675	68.220	−488.377	−401.052	23.276
1000	123.474	494.420	413.913	80.507	−488.487	−391.343	20.442
1100	124.199	506.223	421.776	92.892	−488.663	−381.621	18.122
1200	124.851	517.058	429.271	105.345	−488.911	−371.880	16.188
1300	125.430	527.075	436.414	117.859	−489.224	−362.115	14.550
1400	125.936	536.389	443.226	130.428	−489.598	−352.323	13.145
1500	126.369	545.093	449.730	143.044	−490.033	−342.503	11.927
1600	126.621	553.257	455.948	155.694	−490.535	−332.652	10.860
1700	126.854	560.940	461.900	168.368	−491.111	−322.767	9.917
1800	127.069	568.197	467.606	181.064	−491.759	−312.846	9.079
1900	127.266	575.073	473.083	193.781	−492.480	−302.887	8.327
2000	127.445	581.605	478.347	206.516	−493.274	−292.889	7.649
2100	127.548	587.826	483.413	219.266	−494.147	−282.848	7.035
2200	127.645	593.762	488.295	232.026	−495.102	−272.764	6.476
2300	127.738	599.438	493.005	244.795	−496.143	−262.635	5.965
2400	127.825	604.876	497.554	257.573	−597.789	−250.321	5.448
2500	127.907	610.096	501.952	270.360	−599.162	−235.815	4.927
2600	127.984	615.114	506.208	283.155	−600.561	−221.254	4.445
2700	128.056	619.946	510.332	295.957	−601.989	−206.637	3.998
2800	128.122	624.604	514.330	308.766	−603.448	−191.968	3.581
2900	128.184	629.101	518.211	321.581	−604.939	−177.246	3.193
3000	128.240	633.448	521.980	334.402	−606.464	−162.473	2.829
3100	128.273	637.653	525.644	347.228	−608.022	−147.647	2.488
3200	128.305	641.726	529.208	360.057	−609.615	−132.771	2.167
3300	128.336	645.675	532.678	372.889	−611.241	−117.844	1.865
3400	128.365	649.506	536.058	385.724	−612.897	−102.869	1.580
3500	128.393	653.228	539.353	398.562	−614.580	−87.843	1.311
3600	128.419	656.845	542.567	411.402	−616.287	−72.769	1.056
3700	128.444	660.364	545.703	424.245	−618.014	−57.648	0.814
3800	128.468	663.790	548.766	437.091	−619.756	−42.480	0.584
3900	128.491	667.127	551.758	449.939	−621.509	−27.266	0.365
4000	128.512	670.380	554.683	462.789	−623.268	−12.006	0.157
4100	128.527	673.554	557.544	475.641	−625.027	3.298	−0.042
4200	128.543	676.651	560.343	488.495	−1586.482	32.692	−0.407
4300	128.557	679.676	563.083	501.350	−1586.054	71.239	−0.865
4400	128.572	682.632	565.767	514.206	−1585.615	109.775	−1.303
4500	128.585	685.521	568.396	527.064	−1585.161	148.302	−1.721
4600	128.598	688.347	570.973	539.923	−1584.688	186.818	−2.121
4700	128.611	691.113	573.500	552.784	−1584.192	225.323	−2.504
4800	128.623	693.821	575.978	565.645	−1583.669	263.819	−2.871
4900	128.635	696.473	578.410	578.508	−1583.116	302.302	−3.223
5000	128.645	699.072	580.798	591.372	−1582.530	340.774	−3.560
5100	128.656	701.620	583.142	604.237	−1581.908	379.234	−3.884
5200	128.666	704.118	585.444	617.103	−1581.248	417.681	−4.196
5300	128.675	706.569	587.707	629.970	−1580.547	456.116	−4.495
5400	128.684	708.974	589.930	642.838	−1579.806	494.537	−4.784
5500	128.692	711.336	592.116	655.707	−1579.021	532.944	−5.061
5600	128.700	713.655	594.266	668.577	−1578.192	571.335	−5.329
5700	128.707	715.933	596.381	681.447	−1577.318	609.712	−5.587
5800	128.713	718.171	598.461	694.318	−1576.399	648.073	−5.837
5900	128.719	720.371	600.509	707.190	−1575.435	686.418	−6.077
6000	128.725	722.535	602.525	720.062	−1574.424	724.745	−6.309

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Difluoroborane ((BF$_2$)$_2$) IDEAL GAS M_r = 97.613612 Difluoroborane ((BF$_2$)$_2$) B$_2$F$_4$(g)

$S°$(298.15 K) = [318.47] J·K^{-1}·mol^{-1}

$\Delta_fH°$(0 K) = Unknown
$\Delta_fH°$(298.15 K) = −1431.8 ± 4.2 kJ·mol^{-1}

Vibrational Frequencies and Degeneracies		
υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}
1380 (1)	1155(1)	325(1)
[630](1)	542(1)	1378(1)
[304](1)	1386(1)	662(1)
Rotation	657(1)	325(1)

Ground State Quantum Weight: 1 σ = 4
Point Group: D$_{2d}$
Bond Distances: B–B = 1.67 Å; B–F = 1.32 Å
Bond Angles: F–B–F = 120°; F–B–B = 120°
Dihedral angle between two BF$_2$ planes = 90°
Product of the Moments of Inertia: $I_AI_BI_C$ = 2.502146 × 10^{-113} g^3·cm^6

Enthalpy of Formation

The enthalpy of formation was calculated based on the value, $\Delta_rH°$ = −82.0 ± 1.0 kcal·mol^{-1} for the reaction $B_2F_4(g) + Cl_2(g) = 0.92\ BF_3(g) + 0.46\ BF_2Cl(g) + 0.32\ BFCl_2(g) + 0.30\ BCl_3(g)$ reported by Gunn and Green.[1]

Heat Capacity and Entropy

The molecular and spectroscopic constants were obtained from Gayles and Self.[2] The vibrational frequencies were corrected to the average isotropic species. The molecular configuration was reported to be staggered, analogous to that observed for B$_2$Cl$_4$(g). The angle between two B–BF$_2$ planes is approximately 90°. The thermodynamic functions were evaluated based on an assumption that there is free rotation at the B–B bond. The reduced moment of inertia for the BF$_2$ top is I_r = 4.1231 × 10^{-39} g·cm^2. The principal moments of inertia are: I_A = 16.4908 × 10^{-39}, $I_B = I_C$ = 38.9529 × 10^{-39} g·cm^2

References

[1] S. R. Gunn and L. G. Green, J. Phys. Chem. 65, 178 (1961).
[2] J. N. Gayles and J. Self, J. Chem. Phys. 40, 3530 (1964).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K$_f$
0							
100	43.322	255.051	376.204	−12.115	−1429.664	−1421.034	742.272
200	61.947	290.817	325.053	−6.847	−1430.920	−1411.855	368.739
250	70.075	305.535	319.702	−3.542	−1431.362	−1407.037	293.984
298.15	76.891	318.473	318.473	0.	−1431.765	−1402.315	245.680
300	77.135	318.950	318.475	0.142	−1431.780	−1402.133	244.133
350	83.308	331.314	319.437	4.157	−1432.198	−1397.158	208.514
400	88.716	342.799	321.648	8.461	−1432.626	−1392.124	181.793
450	93.438	353.528	324.601	13.017	−1433.059	−1387.035	161.003
500	97.541	363.590	328.002	17.794	−1433.485	−1381.898	144.366
600	104.163	381.988	335.496	27.895	−1434.294	−1371.504	119.400
700	109.105	398.435	343.334	38.571	−1435.032	−1360.979	101.558
800	112.815	413.257	351.163	49.675	−1435.712	−1350.354	88.169
900	115.634	426.715	358.822	61.104	−1436.355	−1339.645	77.751
1000	117.806	439.016	366.235	72.781	−1436.982	−1328.866	69.413
1100	119.505	450.327	373.372	84.650	−1437.613	−1318.024	62.588
1200	120.855	460.785	380.227	96.670	−1438.262	−1307.123	56.898
1300	121.940	470.503	386.802	108.812	−1438.942	−1296.168	52.081
1400	122.824	479.573	393.108	121.051	−1439.663	−1285.159	47.950
1500	123.553	488.073	399.158	133.371	−1440.433	−1274.096	44.368
1600	124.161	496.067	404.968	145.758	−1441.256	−1262.980	41.232
1700	124.671	503.610	410.551	158.200	−1442.137	−1251.811	38.463
1800	125.104	510.748	415.921	170.690	−1443.077	−1240.589	36.001
1900	125.475	517.522	421.091	183.219	−1444.074	−1229.313	33.796
2000	125.794	523.967	426.075	195.783	−1445.127	−1217.982	31.810
2100	126.070	530.111	430.884	208.376	−1446.233	−1206.598	30.012
2200	126.311	535.982	435.529	220.996	−1447.387	−1195.160	28.377
2300	126.523	541.601	440.019	233.638	−1448.583	−1183.668	26.882
2400	126.710	546.990	444.365	246.300	−1550.335	−1169.986	25.464
2500	126.875	552.166	448.574	258.979	−1551.754	−1154.109	24.114
2600	127.023	557.145	452.655	271.674	−1553.134	−1138.176	22.866
2700	127.154	561.941	456.614	284.383	−1554.468	−1122.191	21.710
2800	127.273	566.568	460.459	297.104	−1555.751	−1106.157	20.636
2900	127.379	571.036	464.195	309.837	−1556.980	−1090.078	19.634
3000	127.475	575.356	467.829	322.580	−1558.150	−1073.958	18.699
3100	127.563	579.537	471.366	335.332	−1559.257	−1057.800	17.824
3200	127.642	583.588	474.810	348.092	−1560.299	−1041.607	17.002
3300	127.715	587.517	478.166	360.860	−1561.272	−1025.383	16.230
3400	127.781	591.331	481.438	373.635	−1562.176	−1009.130	15.503
3500	127.842	595.036	484.631	386.416	−1563.008	−992.851	14.817
3600	127.898	598.638	487.748	399.203	−1563.768	−976.550	14.169
3700	127.949	602.143	490.793	411.996	−1564.455	−960.229	13.556
3800	127.997	605.556	493.768	424.793	−1565.069	−943.890	12.975
3900	128.040	608.881	496.678	437.595	−1565.610	−927.536	12.423
4000	128.081	612.124	499.523	450.401	−1566.079	−911.169	11.899
4100	128.119	615.287	502.308	463.211	−1566.475	−894.791	11.400
4200	128.154	618.374	505.035	476.025	−2526.500	−864.356	10.750
4300	128.187	621.390	507.706	488.842	−2524.581	−824.804	10.019
4400	128.218	624.338	510.324	501.662	−2522.597	−785.297	9.323
4500	128.246	627.219	512.889	514.485	−2520.551	−745.836	8.657
4600	128.273	630.038	515.406	527.311	−2518.443	−706.421	8.022
4700	128.298	632.797	517.874	540.140	−2516.276	−667.052	7.413
4800	128.322	635.499	520.296	552.971	−2514.052	−627.730	6.831
4900	128.344	638.145	522.675	565.804	−2511.773	−588.456	6.273
5000	128.365	640.738	525.010	578.639	−2509.442	−549.228	5.738
5100	128.384	643.280	527.304	591.477	−2507.060	−510.047	5.224
5200	128.403	645.773	529.559	604.316	−2504.631	−470.913	4.730
5300	128.420	648.219	531.774	617.157	−2502.156	−431.827	4.256
5400	128.437	650.620	533.953	630.000	−2499.638	−392.788	3.799
5500	128.452	652.977	536.096	642.845	−2497.079	−353.796	3.360
5600	128.467	655.291	538.204	655.691	−2494.481	−314.850	2.937
5700	128.481	657.565	540.278	668.538	−2491.847	−275.952	2.529
5800	128.495	659.800	542.319	681.387	−2489.178	−237.100	2.135
5900	128.507	661.997	544.329	694.237	−2486.478	−198.294	1.756
6000	128.519	664.157	546.308	707.088	−2483.748	−159.535	1.389

PREVIOUS December 1964 (1 atm)   CURRENT. December 1964 (1 bar)

Difluoroborane Oxide ($O(BF_2)_2$) IDEAL GAS $M_r = 113.613012$

$S°(298.15\ K) = [337.52 + 8.4]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K)$ = Unknown

$\Delta_f H°(298.15\ K) = -1898.07 + 8.4\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
[1400](1)	[145](1)	[1370](1)
[670](1)	[800](1)	[145](1)
[320](1)	[660](1)	[1800](1)
rotation	[660](1)	[1155](1)
[1370](1)	[1600](1)	[540](1)

Ground State Quantum Weight: 1 $\sigma = 4$

Point Group: D_{2h}

Bond Distances: B–O = [1.4] Å; B–F = [1.32] Å

Bond Angles: B–O–B = [180]°; F–B–F = [120]°

Dihedral angle between the two BF_2 planes = 90°

Product of the Moments of Inertia: $I_A I_B I_C = [7.701231 \times 10^{-113}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

Bidinosti and Coatsworth[1] have reported $\Delta_r H°(1100\ K) = 18.5 \pm 3\ kcal{\cdot}mol^{-1}$ for the reaction $4\ BF_3(g) + B_2O_3(l) = 3\ B_2OF_4(g)$. This value was obtained from a mass spectrometric study of the variation of the ion intensities with temperature of the BF_3^+ and $B_2OF_4^+$ species. Employing JANAF auxiliary values[2] we obtain $\Delta_f H°(B_2F_4O,\ g,\ 1100\ K) = -455.75 \pm 2\ kcal{\cdot}mol^{-1}$ which reduces to $\Delta_f H°(298.15\ K) = -453.65 \pm 2\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

By analogy with $B_2F_4(g)$[3] free rotation of the BF_2 groups is assumed. Because of the large separation of the two BF_2 groups the molecule is considered to be planar. The B–O distance is assumed to be that in $BF_2O(g)$[2] and the B–F distance that in $B_2F_4(g)$.[2] The vibrational frequencies are estimated by comparison with those for B_2F_4;[3] the values are given above in the order $3A_g$, A_u, $2B_{1g}$, $2B_{1u}$, B_{2g}, $3B_{2u}$, $3B_{3u}$. The thermodynamic functions were evaluated based on an assumption that there is free rotation at the two B–O bonds. The reduced moment of inertia for the BF_2 top is $I_r = 4.1227 \times 10^{-39}\ g{\cdot}cm^2$. The principal moments of inertia are: $I_A = 16.4908 \times 10^{-39}$, $I_B = 60.5877 \times 10^{-39}$, and $I_C = 77.0785 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] D. R. Bidinosti and L. L. Coatsworth, Can. J. Chem. 48, 2484 (1970).

[2] JANAF Thermochemical Tables: $BF_3(g)$, 6–30–69; $B_2O_3(l)$, 6–30–71; $BF_2O(g)$, 12–31–66; $B_2F_4(g)$, 12–31–64.

[3] L. A. Nimon, K. S. Seshadri, D. White and R. C. Taylor, AD–693614, (1969).

Difluoroborane Oxide ($O(BF_2)_2$) $B_2F_4O_1(g)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K_f
0							
100	51.315	267.752	399.768	−13.202	−1894.168	−1878.142	981.041
200	66.790	307.999	344.533	−7.307	−1896.253	−1861.276	486.115
250	74.652	323.753	338.831	−3.770	−1897.191	−1852.422	387.042
298.15	81.853	337.523	337.523	0.	−1898.072	−1843.720	323.012
300	82.121	338.031	337.525	0.152	−1898.105	−1843.382	320.961
350	89.101	351.220	338.551	4.434	−1898.993	−1834.191	273.738
400	95.547	363.545	340.913	9.053	−1899.853	−1824.875	238.304
450	101.427	375.144	344.078	13.980	−1900.674	−1815.453	210.732
500	106.733	386.110	347.738	19.186	−1901.443	−1805.942	188.665
600	115.686	406.393	355.852	30.325	−1902.793	−1786.711	155.547
700	122.698	424.775	364.406	42.258	−1903.900	−1767.273	131.876
800	128.153	441.531	373.015	54.812	−1904.799	−1747.692	114.113
900	132.412	456.881	381.493	67.849	−1905.537	−1728.007	100.291
1000	135.763	471.012	389.748	81.265	−1906.157	−1708.248	89.230
1100	138.428	484 082	397.737	94.979	−1906.696	−1688.430	80.177
1200	140.570	496.222	405.444	108.933	−1907.187	−1668.566	72.631
1300	142.311	507.544	412.868	123.080	−1907.653	−1648.662	66.244
1400	143.742	518.145	420.013	137.385	−1908.116	−1628.722	60.768
1500	144.929	528.104	426.890	151.820	−1908.591	−1608.749	56.022
1600	145.923	537.490	433.512	166.364	−1909.090	−1588.743	51.867
1700	146.763	546.362	439.892	180.999	−1909.624	−1568.706	48.200
1800	147.479	554.772	446.043	195.712	−1910.197	−1548.635	44.940
1900	148.093	562.762	451.977	210.492	−1910.815	−1528.532	42.022
2000	148.623	570.372	457.708	225.328	−1911.477	−1508.395	39.395
2100	149.084	577.635	463.247	240.214	−1912.183	−1488.224	37.018
2200	149.487	584.580	468.606	255.143	−1912.931	−1468.018	34.855
2300	149.841	591.233	473.794	270.110	−1913.718	−1447.777	32.880
2400	150.154	597.617	478.821	285.110	−2015.058	−1425.363	31.022
2500	150.432	603.752	483.696	300.139	−2016.065	−1400.772	29.268
2600	150.679	609.657	488.428	315.195	−2017.031	−1376.141	27.647
2700	150.901	615.348	493.024	330.274	−2017.954	−1351.474	26.146
2800	151.100	620.840	497.492	345.375	−2018.827	−1326.773	24.751
2900	151.280	626.145	501.837	360.494	−2019.648	−1302.042	23.452
3000	151.442	631.277	506.067	375.630	−2020.413	−1277.284	22.239
3100	151.590	636.245	510.186	390.782	−2021.118	−1252.501	21.105
3200	151.724	641.060	514.201	405.948	−2021.762	−1227.697	20.040
3300	151.847	645.730	518.116	421.126	−2022.340	−1202.873	19.040
3400	151.959	650.265	521.937	436.317	−2022.852	−1178.033	18.098
3500	152.062	654.672	525.667	451.518	−2023.296	−1153.179	17.210
3600	152.156	658.957	529.310	466.729	−2023.672	−1128.313	16.371
3700	152.244	663.127	532.870	481.949	−2023.978	−1103.437	15.578
3800	152.324	667.188	536.352	497.177	−2024.215	−1078.555	14.826
3900	152.399	671.146	539.758	512.413	−2024.383	−1053.666	14.112
4000	152.468	675.005	543.091	527.657	−2024.482	−1028.774	13.434
4100	152.532	678.770	546.354	542.907	−2024.513	−1003.882	12.790
4200	152.592	682.447	549.551	558.163	−2984.176	−964.940	12.001
4300	152.647	686.038	552.683	573.425	−2981.899	−916.890	11.138
4400	152.699	689.548	555.754	588.692	−2979.561	−868.893	10.315
4500	152.748	692.980	558.766	603.965	−2977.164	−820.950	9.529
4600	152.793	696.338	561.720	619.242	−2974.710	−773.062	8.778
4700	152.836	699.624	564.619	634.523	−2972.202	−725.227	8.060
4800	152.876	702.842	567.466	649.809	−2969.640	−677.445	7.372
4900	152.914	705.995	570.261	665.098	−2967.029	−629.718	6.713
5000	152.949	709.085	573.006	680.392	−2964.371	−582.045	6.081
5100	152.983	712.114	575.704	695.688	−2961.667	−534.425	5.474
5200	153.014	715.085	578.356	710.988	−2958.922	−486.859	4.891
5300	153.044	718.000	580.964	726.291	−2956.136	−439.345	4.330
5400	153.072	720.861	583.528	741.597	−2953.314	−391.886	3.791
5500	153.099	723.670	586.050	756.905	−2950.458	−344.479	3.272
5600	153.124	726.428	588.533	772.216	−2947.571	−297.122	2.771
5700	153.148	729.139	590.976	787.530	−2944.655	−249.820	2.289
5800	153.171	731.803	593.381	802.846	−2941.713	−202.567	1.824
5900	153.192	734.421	595.749	818.164	−2938.749	−155.366	1.376
6000	153.213	736.996	598.082	833.484	−2935.764	−108.215	0.942

PREVIOUS: June 1971 (1 atm) CURRENT: June 1971 (1 bar)

Dihydroxyborane ((B(OH)$_2$)$_2$) CRYSTAL $M_r = 89.64936$ Dihydroxyborane ((B(OH)$_2$)$_2$) $B_2H_4O_4$(cr)

$\Delta_f H°(0\ K)$ = Unknown
$S°(298.15\ K) = [126 \pm 4]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -1410 \pm 8\ kJ{\cdot}mol^{-1}$
T_{fus} = Unknown
$\Delta_{fus} H°$ = Unknown

Enthalpy of Formation

The enthalpy change, $\Delta_r H°(298.15\ K) = -91.3 \pm 1\ kcal{\cdot}mol^{-1}$, for the reaction $B_2(OH)_4(cr) + (m+2)AgNO_3(aq) + (n+2)\ H_2O(l) = 2\ Ag(cr) + [2\ H_1BO_3 + 2\ HNO_3 + mAgNO_3]nH_2O(aq)$ was determined electrically by Finch *et al.*[1] The enthalpy of formation of $B_2(OH)_4$(cr) was reported to be $-335.1\ kcal{\cdot}mol^{-1}$. This value was corrected to be $337.1 \pm 2\ kcal{\cdot}mol^{-1}$ by use of more recent data on the $\Delta_f H°(298.15\ K)$ values used for calculation.

Heat Capacity and Entropy

The heat capacity for $B_2(OH)_4$(cr) was estimated by comparison with those for $B(OH)_3$(cr). $S°(298.15\ K)$ was calculated based on $3\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ per atom for $B_2(OH)_4$(cr), which was obtained from the corresponding values for HBO_2(cr) and $B(OH)_1$(cr).

Sublimation Data

The value, $\Delta_{sub} H°(298.15\ K)$, was as the difference between $\Delta_f H°(298.15\ K)$ for $B_2(OH)_4$(g) and $B_2(OH)_4$(cr).

Reference

[1] A. Finch, P. J. Gardner, and I. J. Hyams, Trans. Faraday Soc. **61**, 649 (1965).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	116.190	125.520	125.520	0.	−1410.426	−1244.118	217.964
300	116.775	126.241	125.522	0.215	−1410.468	−1243.086	216.441
400	143.135	163.582	130.435	13.259	−1411.904	−1187.032	155.010
500	163.762	197.787	140.535	28.626	−1411.962	−1130.781	118.132
600	181.711	229.271	152.735	45.922	−1410.806	−1074.634	93.555
700	197.025	258.456	165.779	64.874	−1408.549	−1018.770	76.022
800	210.413	285.665	179.083	85.266	−1405.302	−963.298	62.897
900	221.459	311.098	192.354	106.869	−1401.222	−908.284	52.715
1000	231.333	334.953	205.434	129.519	−1396.428	−853.764	44.596
1100	239.994	357.417	218.239	153.095	−1391.008	−799.755	37.977
1200	247.442	378.626	230.729	177.476	−1385.059	−746.264	32.484
1300	253.801	398.691	242.885	202.548	−1378.678	−693.287	27.857
1400	258.990	417.697	254.699	228.197	−1371.963	−640.814	23.909
1500	263.006	435.709	266.171	254.307	−1365.021	−588.831	20.505

PREVIOUS: CURRENT: March 1966

Dihydroxyborane ((B(OH)$_2$)$_2$) IDEAL GAS $M_r = 89.64936$ Dihydroxyborane ((B(OH)$_2$)$_2$) B$_2$H$_4$O$_4$(g)

$S°(298.15\ K) = [348.93]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K)$ = Unknown
$\Delta_f H°(298\ 15\ K) = [-1284 \pm 20]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}
[1380](1)	[1386](1)	[824](2)
[630](1)	[657](1)	[209](2)
[304](1)	[325](1)	[3200](4)
Rotation	[1378](1)	[1200](2)
[1155](1)	[662](1)	[880](2)
[542](1)	[325](1)	

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: [C$_2$]
Bond Distances: B–B = [1.67] Å; B–O = [1.36] Å; O–H = [0.96] Å
Bond Angles: H–O–B = [114]°; O–B–O = [120]°; O–B–B = [120]°
Dihedral angle between two B(OH)$_2$ planes = 90°
Product of the Moments of Inertia: $I_A I_B I_C = [2.299983 \times 10^{-113}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpy of formation, $\Delta_f H°(B_2(OH)_4, g, 298.15\ K)$, is calculated using bond energies, $D_0°(B\text{–}OH) = 132$ and $D_0°(B\text{–}B) = 78\ kcal\ mol^{-1}$. The bond energy $D_0°(B\text{–}OH)$ was taken from that in B(OH)$_3$(g) and $D_0°(B\text{–}B)$ was estimated by comparison with that in B$_2$F$_4$(g).

Heat Capacity and Entropy

The molecular structure was assumed to be the same as that for B$_2$F$_4$(g), i.e. the two B(OH)$_2$ units have staggered configuration, and free rotation about B–B bond. The B–B bond distance was taken as that in B$_2$F$_4$ molecule. Those for B–O and B–H bond and bond angles were adopted from H$_3$BO$_3$ molecule. Eleven vibratonal frequencies were assumed to be the same as those for B$_2$F$_4$(g). In addition to these were added four OH torsion frequencies, 824(2) and 209(2), four OH stretching, 3200(4), and four B–O–H bending frequencies, 1200(2) and 880(2). The thermodynamic functions were evaluated based on an assumption that there is free rotation at the B–B bond. The reduced moment of inertia for the B(OH)$_2$ top is $I_r = 4.1012 \times 10^{-39}\ g{\cdot}cm^{-2}$. The principal moments of inertia are: $I_A = 16.4048 \times 10^{-39}$, $I_B = 37.4430 \times 10^{-39}$, and $I_C = 37.4441 \times 10^{-39}\ g{\cdot}cm^2$.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
0							
100	51.574	268.590	423.555	−15.496	−1275.111	−1247.102	651.419
200	78.745	312.793	357.611	−8.964	−1280.454	−1216.886	317.818
250	91.679	331.764	350.567	−4 701	−1282.641	−1200.736	250.880
298.15	103.433	348.929	348.929	0.	−1284.488	−1184.789	207.570
300	103.867	349.571	348.931	0.192	−1284.554	−1184.170	206.182
350	114.997	366.432	350.238	5.668	−1286.183	−1167.307	174.211
400	124.923	382.450	353.272	11.671	−1287.553	−1150.228	150.204
450	133.648	397.679	357.367	18.140	−1288.695	−1132.992	131.514
500	141.275	412.164	362.128	25.018	−1289.632	−1115.639	116.550
600	153.812	439.078	372.747	39.799	−1290.991	−1080.703	94.084
700	163.658	463.556	383.998	55.691	−1291.794	−1045.585	78.022
800	171.644	485.948	395.362	72.469	−1292.160	−1010.383	65.971
900	178.299	506.561	406.588	89.976	−1292.177	−975.156	56.597
1000	183.944	525.646	417.551	108.095	−1291.914	−939.943	49.098
1100	188.786	543.411	428.195	126.738	−1291.427	−904.768	42.964
1200	192.966	560.021	438.496	145.830	−1290.767	−869.645	37.855
1300	196.593	575.613	448.450	165.312	−1289.975	−834.583	33.534
1400	199.750	590.300	458.062	185.133	−1289.089	−799.585	29.833
1500	202.506	604.178	467.345	205.249	−1288.140	−764.654	26.628
1600	204.921	617.326	476.312	225.623	−1287.156	−729.787	23.825
1700	207.043	629.814	484.977	246.224	−1286.158	−694.982	21.354
1800	208.912	641.703	493.356	267.023	−1285.167	−660.236	19.160
1900	210.566	653.043	501.465	287.999	−1284.199	−625.544	17.197
2000	212.032	663.882	509.317	309.130	−1283.268	−590.902	15.433
2100	213.337	674.259	516.926	330.400	−1282.385	−556.305	13.837
2200	214.502	684.211	524.305	351.793	−1281.560	−521.749	12.388
2300	215.545	693.769	531.467	373.296	−1280.802	−487.230	11.065
2400	216.482	702.963	538.422	394.899	−1380.634	−450.605	9.807
2500	217.326	711.818	545.182	416.590	−1380.183	−411.863	8.605
2600	218.089	720.356	551.756	438.361	−1379.750	−373.139	7.496
2700	218.779	728.600	558.154	460.205	−1379.339	−334.430	6.470
2800	219.406	736.568	564.384	482.115	−1378.953	−295.736	5.517
2900	219.977	744.278	570.455	504.084	−1378.597	−257.058	4.630
3000	220 498	751.744	576.375	526.109	−1378.271	−218.389	3.802
3100	220.975	758.982	582.149	548.183	−1377.978	−179.730	3.028
3200	221.412	766.005	587.785	570.302	−1377.720	−141.083	2.303
3300	221.814	772.824	593.290	592.464	−1377.497	−102.442	1.622
3400	222.184	779.452	598.668	614.664	−1377.311	−63.806	0.980
3500	222.525	785.897	603.926	636.900	−1377.163	−25.176	0.376
3600	222.841	792.170	609.068	659.168	−1377.053	13.451	−0.195
3700	223.133	798.280	614.100	681.467	−1376.981	52.074	−0.735
3800	223.404	804.234	619.025	703.794	−1376.950	90.699	−1.247
3900	223.656	810.041	623.849	726.147	−1376.957	129.321	−1.732
4000	223.890	815.706	628.575	748.525	−1377.005	167.943	−2.193
4100	224.109	821.237	633.207	770.925	−1377.094	206.568	−2.632
4200	224.313	826.640	637.748	793.346	−2336.923	259.244	−3.224
4300	224.504	831.921	642.203	815.787	−2334.920	321.035	−3.900
4400	224.682	837.084	646.573	838.246	−2332.962	382.777	−4.544
4500	224.850	842.135	650.863	860.723	−2331.051	444.476	−5.159
4600	225.007	847.079	655.075	883.216	−2329.187	506.133	−5.747
4700	225.155	851.919	659.212	905.724	−2327.371	567.751	−6.310
4800	225.294	856.661	663.276	928.247	−2325.605	629.331	−6.849
4900	225.425	861.308	667.271	950.783	−2323.889	690.875	−7.365
5000	225.548	865.863	671.197	973.331	−2322.225	752.385	−7.860
5100	225.665	870.331	675.058	995.892	−2320.613	813.861	−8.336
5200	225.775	874.714	678.856	1018.464	−2319.054	875.304	−8.793
5300	225.880	879.016	682.592	1041.047	−2317.551	936.722	−9.232
5400	225.978	883.239	686.268	1063 640	−2316.104	998.108	−9.655
5500	226.072	887.386	689.888	1086.242	−2314.714	1059.468	−10.062
5600	226.161	891.460	693.451	1108.854	−2313.383	1120.807	−10.454
5700	226.245	895.464	696.960	1131.474	−2312.112	1182.120	−10.833
5800	226.325	899.400	700.416	1154.103	−2310.902	1243.413	−11.198
5900	226.401	903.269	703.822	1176.739	−2309.754	1304.680	−11.551
6000	226.474	907.075	707.178	1199.383	−2308.671	1365.935	−11.892

PREVIOUS: March 1966 (1 atm) CURRENT: March 1966 (1 bar)

Diborane(B_2H_6) IDEAL GAS $M_r = 27.66764$ Diborane (B_2H_6) $B_2H_6(g)$

$S°(298.15\ K) = 233.17\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 56.7 \pm 16.7\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 41.0 \pm 16.7\ kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies			
υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}
2532(1)	2600(1)	1026(1)	2615(1)
2109(1)	919(1)	584(1)	1601(1)
1184(1)	1755(1)	1905(1)	1174(1)
788(1)	942(1)	973(1)	
2612(1)	950(1)	368(1)	

Ground State Quantum Weight: [1] $\sigma = 4$
Point Group: D_{2h}
Bond Distances: B–B = 1 775 ± 0.004 Å; $B–H_t = 1.196 \pm 0.016$ Å; $B–H_b = 1.339 \pm 0.013$ Å
H_t = terminal hydrogen, H_b = bridge hydrogens.
Bond Angles: $H_t–B–H_t = 120.2 \pm 1.6°$
Product of the Moments of Inertia: $I_AI_BI_C = 2.459830 \times 10^{116}\ g^3·cm^6$

Enthalpy of Formation

$\Delta_f H°(298.15\ K)$ is a weighted average of the following data. The older data of Roth *et al.*[8] deviates from the rest of the investigations and is not included.

Source	Reaction	$\Delta_r H°(298.15\ K)$ kcal·mol^{-1}	$\Delta_f H°(298.15\ K)$ kcal·mol^{-1}
1	$B_2H_6(g) \rightarrow 2\ B(am) + 3\ H_2(g)$	−5.0	7.4
2	$B_2H_6(g) \rightarrow 2\ B(am) + 3\ H_2(g)$	−6.73	9.13
3	$B_2H_6(g) + 6\ Cl_2 \rightarrow 2\ BCl_3(g) + 6\ HCl(g)$	−342.3	17.3
4	$B_2H_6(g) + 6\ H_2O(l) + [2000\ H_2O](l) \rightarrow$ $2[H_3BO_3 + 1000\ H_2O](soln) + 6\ H_2(g)$	−111.46 ± 0.54	9.32
7a	$B_2H_6(g) + 2006\ H_2O \rightarrow 2(H_3BO_3 + 1000\ H_2O) + 6\ H_2(g)$	−112.22 ± 0.10	10.08
7b	$BCl_3(l) + 130.3\ H_2O \rightarrow (H_3BO_3 + 1000\ H_2O) + 3(HCl + 100\ H_2O)$	−68.14	—
(a)−2(b)−(c)	$B_2H_6(g) + 6(HCl100\ H_2O) \rightarrow 2\ BCl(l) + 6\ H_2(g)$	+24.06	10.06
9	$(CH_3)_3\ N(g) + 1/2\ B_2H_6(g) \rightarrow (CH_3)_3N{:}BH_3(cr)$	−32.33 ± 0.06	8.3
13	$(CH_3)_3N(g) + 1/2\ B_2H_6(g) \rightarrow CH_3)_3N{:}BH_3(cr)$	−31.40	6.5

Sources of Auxiliary Data: From the JANAF tables, $\Delta_f H°(298.15\ K) = 1.2, -96.31, -22.063$ kcal mol^{-1} of B(am), $BCl_3(g)$ and HCl(g), respectively. From Rossini,[11] the $\Delta_{vap}H°(298.15\ K) = 5.6$ kcal·mol^{-1} of BCl_3. From Wagman,[12] the $\Delta_f H°(298.15\ K)$ of $(HCl + 1000\ H_2O) = -39.657$ kcal·mol^{-1}. From Good *et al.*,[5] the $\Delta_f H°(H_3BO_3,\ cr,\ 298.15\ K) = -261.47 \pm 0.20$ kcal·mol^{-1} and the H_3BO_3 solution data of Fasolino.[6] $\Delta_f H°((CH_3)_3N,\ g,\ 298.15\ K) = -5.9 \pm 0.4$ kcal·mol^{-1} from Jaffe.[10]

Heat Capacity and Entropy

The molecular constants reported by Carroll,[14] were selected. They agree well with those reported by Hedberg and Schomaker.[15] The principal moments of inertia are $I_A = 1.0562 \times 10^{-39}$, $I_B = 4.6381 \times 10^{-39}$, and $I_C = 5.0213 \times 10^{-39}\ g·cm^2$.

The vibrational frequencies for $B_2{}^{11}H_6$ were those listed by Wu[16] except for υ_8, υ_{10} and υ_{14} which were taken from the calculated frequency column of Table VIII–1 (page 55) of the Thesis.

References

[1] S. R. Gunn and L. G. Green, J. Phys. Chem. 65, 779 83 (1961); J. Chem. Phys. 36, 1118 (1962). Explosive decomposition while mixed with stibine.

[2] E. J. Prosen, W. H. Johnson and F. Y. Pergiel, J. Res. Nat. Bur. Stand. 61, 247 250 (1958). Decomposition by heating in a flow type calorimeter.

[3] J. R. Lacher, R. E. Scruby, and J. D. Park, J. Am. Chem. Soc. 74, 5292 4 (1952) A vapor phase chlorination in a flow type calorimeter.

[4] E. J. Prosen, W. H. Johnson, and F. Y. Pergiel, J. Res. Nat. Bur. Stand. 62, 43 47 (1959). Heat of reaction of diborane with water in a flow type calorimeter.

[5] W. D. Good, M. Mansson, and J. P. McCullough, Thermochemistry of Boron and Some of its Compoudns. The heats of Formation of Trimethylamineborane and Orthaboric Acid, Symp. on Thermodynamics and Thermochemistry, Lund, Sweden, (July 1963).

Continued on page 317

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−12.149	56.684	56.684	INFINITE
100	34.592	186.917	274.911	−8.799	50.988	62.576	−32.686
200	43.499	213.191	237.985	−4.959	46.081	76.058	−19.864
250	50.526	223.629	234.083	−2.613	43.496	83.850	−17.519
298.15	58.100	233.170	233.170	0.	41.003	91.849	−16.092
300	58.397	233.530	233.171	0.108	40.909	92.165	−16.047
350	66.435	243.137	233.911	3.229	38.429	100.905	−15.059
400	74.255	252.522	235.653	6.748	36.106	109.991	−14.363
450	81.690	261 701	238.039	10.648	33.970	119.357	−13.855
500	88.683	270.674	240.856	14.909	32.037	128.950	−13.471
600	101.331	287.988	247.280	24.425	28.803	148.650	−12.941
700	112.275	304.451	254.282	35.119	26.373	168.828	−12.598
800	121.655	320.072	261.538	46.827	24.659	189.303	−12.360
900	129.635	334.875	268.871	59.403	23.547	209.956	−12.186
1000	136.394	348.893	276.179	72.714	22.922	230.706	−12.051
1100	142.112	362.168	283.398	86.647	22.678	251.499	−11.943
1200	146.952	374.747	290.491	101.107	22.725	272.300	−11.853
1300	151.059	386.676	297.435	116 013	22.986	293.089	−11.776
1400	154.558	398.002	304.217	131.298	23.400	313.851	−11.710
1500	157.550	408.770	310.832	146.908	23.917	334.580	−11.651
1600	160.122	419.022	317.276	162.794	24.497	355.272	−11.598
1700	162.342	428.798	323.551	178.920	25.110	375.927	−11.551
1800	164.269	438 133	329.659	195.253	25.732	396.546	−11.507
1900	165.949	447.060	335.605	211.766	26.343	417.130	−11.468
2000	167.421	455.611	341.393	228.436	26.928	437.682	−11.431
2100	168.716	463.811	347.028	245.244	27.475	458.206	−11.397
2200	169.860	471.687	352.517	262.174	27.975	478.705	−11.366
2300	170.876	479.260	357.864	279.212	28.418	499.183	−11.337
2400	171.780	486.552	363.075	296.345	−71.719	521.780	−11.356
2500	172.589	493.581	368.155	313.565	−71.560	546.506	−11.419
2600	173.315	500.365	373.111	330.861	−71.407	571.225	−11.476
2700	173.969	506.918	377.946	348.225	−71.265	595.939	−11.529
2800	174.559	513.256	382.666	365.652	−71.137	620.648	−11.578
2900	175.094	519.391	387.275	383.135	−71.025	645.353	−11.624
3000	175.581	525.335	391.779	400.669	−70.932	670.054	−11.667
3100	176.023	531.100	396.180	418.250	−70.862	694.752	−11.706
3200	176.428	536.695	400.485	435.873	−70.815	719.448	−11.744
3300	176.798	542.130	404.695	453.534	−70.793	744.144	−11.779
3400	177.139	547.413	408.815	471.232	−70.799	768.839	−11.812
3500	177.451	552.552	412.849	488.961	−70.834	793.535	−11.843
3600	177.740	557.555	416.799	506.721	−70.899	818.232	−11.872
3700	178.006	562.429	420.670	524.509	−70.996	842.931	−11.900
3800	178.253	567.179	424.463	542.322	−71.125	867.634	−11.926
3900	178.482	571.812	428.182	560.159	−71.288	892.340	−11.952
4000	178.694	576.334	431.829	578.017	−71.486	917.050	−11.975
4100	178.892	580.749	435.408	595.897	−71.719	941.767	−11.998
4200	179.076	585.062	438.920	613 795	−1031.687	980.538	−12.195
4300	179.248	589.278	442.368	631.712	−1029.819	1028.426	−12.493
4400	179.409	593.400	445.754	649.645	−1027.991	1076.270	−12.777
4500	179.559	597.434	449.080	667.593	−1026.205	1124.074	−13.048
4600	179 700	601.382	452.348	685.556	−1024.461	1171.838	−13.307
4700	179.833	605.248	455.560	703.533	−1022.759	1219.566	−13.554
4800	179.957	609.035	458.718	721.522	−1021.099	1267.258	−13.791
4900	180.075	612.747	461.824	739.524	−1019.481	1314.914	−14.017
5000	180.185	616.386	464.879	757.537	−1017.906	1362.540	−14.234
5100	180.289	619.955	467.885	775.561	−1016.373	1410.133	−14.443
5200	180.387	623.457	470.843	793.595	−1014.881	1457.697	−14.643
5300	180.480	626.894	473.755	811.638	−1013.430	1505.233	−14.835
5400	180.568	630.269	476.622	829.691	−1012.018	1552.742	−15.020
5500	180.651	633.583	479.446	847.752	−1010.645	1600.224	−15.198
5600	180.730	636.838	482.228	865.821	−1009.310	1647.683	−15.369
5700	180.805	640.038	484.968	883.898	−1008.010	1695.118	−15.534
5800	180.876	643.183	487.669	901.982	−1006.745	1742.530	−15.693
5900	180.944	646.276	490.331	920.073	−1005.513	1789.920	−15.847
6000	181.008	649.317	492.956	938.170	−1004.313	1837.290	−15.995

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Magnesium Boride (MgB$_2$) CRYSTAL $M_r = 45.925$ Magnesium Boride (MgB$_2$) B$_2$Mg$_1$(cr)

$S°(298.15\ K) = 35.98 \pm 0.17\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{dcm} = [1320]\ K$

$\Delta_f H°(0\ K) = -91.3 \pm 8.4\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -92.0 \pm 8.4\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The equilibrium constants (993–1108 K) for the reaction 2 MgB$_2$(cr) = Mg(g) + MgB$_4$(cr) were determined by Wright and Walsh.[1] The corresponding 2nd and 3rd law values of $\Delta_r H°(298.15\ K)$ for this reaction were derived as 53.1 ± 4.7 and 54.1 kcal·mol^{-1}, respectively. Using the 3rd law value obtained, i.e., $\Delta_r H°(298.15\ K) = 54.1\ kcal \cdot mol^{-1}$, for the reaction, $\Delta_f H°$(MgB$_2$, cr, 298.15 K) was evaluated as −22.0 ± 2.0 kcal·mol^{-1}.

Heat Capacity and Entropy

The low temperature (21.12–304.22 K) heat capacities were measured by Swift and White[2] Above 298.15 K, the values of C_p were estimated with those of other related borides. $S°(298.15\ K)$ was reported by Swift and White[2] using $S°(\text{extrap}, 20\ K) = 0.005\ cal \cdot K^{-1} \cdot mol^{-1}$.

Decomposition Data

T_{dcm} was taken from Markovsky *et al.*[3] On heating to high temperatures, MgB$_2$(cr) decomposes into boride phases, A, B, and C with the separation of Mg. The composition of phase A is close to MgB$_6$ and that of C is close to MgB$_{12}$.

References

[1] M. Wright and P. N. Walsh, The Vaporization of MgB$_4$(cr), Ohio State University Research Foundation, Tech. Research Report OMCC–HEF–55 (1958).
[2] R. M. Swift and D. White, J. Am. Chem. Soc. 79, 3641 (1957).
[3] L. Y. Markovsky, Y. D. Kondrashev, and G. V. Kaputovskaya, Zhur. Obshchei Khim. 25, 409 (1955).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.799	−91.337	−91.337	INFINITE
100	11.171	4.025	68.961	−6.494	−91.722	−91.112	47.592
200	34.392	19.205	40.125	−4.184	−92.085	−90.330	23.592
298.15	47.823	35.982	35.982	0.	−91.964	−89.473	15.675
300	47.865	36.278	35.983	0.089	−91.964	−89.457	15.576
400	54.392	51.002	37.946	5.222	−92.110	−88.609	11.571
500	58.409	63.590	41.848	10.871	−92.590	−87.684	9.160
600	61.379	74.507	46.402	16.863	−93.328	−86.638	7.542
700	64.015	84.168	51.120	23.134	−94.239	−85.452	6.377
800	66.526	92.879	55.804	29.660	−95.267	−84.128	5.493
900	69.162	100.867	60.373	36.445	−96.364	−82.670	4.798
1000	71.714	108.288	64.798	43.490	−106.100	−80.376	4.198
1100	74.078	115.233	69.070	50.779	−107.301	−77.744	3.692
1200	76.442	121.780	73.193	58.305	−108.384	−75.008	3.265
1300	78.795	127.992	77.171	66.067	−109.336	−72.188	2.901
1400	81.170	133.918	81.014	74.065	−237.558	−66.131	2.467
1500	83.643	139.603	84.732	82.307	−236.863	−53.910	1.877
1600	85.981	145.077	88.333	90.789	−236.012	−41.740	1.363
1700	88.162	150.355	91.827	99.497	−235.015	−29.628	0.910
1800	90.249	155.454	95.221	108.419	−233.881	−17.578	0.510
1900	92.242	160.387	98.522	117.544	−232.618	−5.595	0.154
2000	94.140	165.167	101.735	126.864	−231.232	6.318	−0.165

PREVIOUS: March 1963 CURRENT: March 1965

Boron Oxide (B_2O) IDEAL GAS $M_r = 37.6194$ Boron Oxide (B_2O) $B_2O_1(g)$

$S°(298.15\ K) = [227.7]\ J·K^{-1}·mol^{-1}$

$\Delta_fH°(0\ K) = 93 \pm 105\ kJ·mol^{-1}$
$\Delta_fH°(298.15\ K) = 96 \pm 105\ kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}
[1250](1)
[600](1)
[1800](1)

Ground State Quantum Weight: [1] $\sigma = [2]$
Point Group: [C_{2v}]
Bond Distance: B–O = [1.26] Å
Bond Angle: B–O–B = [150]°
Product of the Moments of Inertia: $I_AI_BI_C = [4.732389 \times 10^{-117}]\ g^3·cm^6$

Enthalpy of Formation

The enthalpy of formation was calculated from the estimated enthalpy of reaction $\Delta_rH°(0\ K) = 300 \pm 25\ kcal·mol^{-1}$ for $B_2O(g) \rightarrow 2B(g) + O(g)$, using the JANAF auxiliary data[2] for B(g) and O(g). The value of $\Delta_rH°(0\ K)$ was assumed to be the sum of the enthalpies of dissociation, 120 $kcal·mol^{-1}$ for $B_2O(g) \rightarrow BO(g) + B(g)$ and 180 $kcal·mol^{-1}$ for $BO(g) \rightarrow B(g) + O(g)$. The former was estimated and the latter was derived from the JANAF values.[2]

The possible existence of $B_2O(g)$ in the burning of boron under reducing conditions was discussed by Bahn.[1] He estimated the enthalpy of formation to lie between −27 and +23 $kcal·mol^{-1}$ but favored the value of +23 $kcal·mol^{-1}$ in the theoretical calculations of boron burning in air.

Heat Capacity and Entropy

The bent molecular structure and the molecular constants were estimated by comparison with those in BO(g), AlO(g) and $Al_2O(g)$. The principal moments of inertia are $I_A = 0.1624 \times 10^{-39}$, $I_B = 5.3179 \times 10^{-39}$, and $I_C = 5.4803 \times 10^{-39}\ g·cm^2$.

References

[1] G. S. Bahn, Combustion Institute, University of Denver (1966).
[2] JANAF Thermochemical Tables: B(g), 12–31–64; and O(g), 6–30–62.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−10.375	92.626	92.626	INFINITE
100	33.368	189.391	259.874	−7.048	94.453	84.241	−44.003
200	35.469	213.037	231.161	−3.625	95.755	73.464	−19.187
250	36.956	221.110	228.368	−1.814	96.094	67.847	−14.176
298.15	38.410	227.744	227.744	0.	96.232	62.391	−10.931
300	38.466	227.982	227.745	0.071	96.234	62.181	−10.827
350	39.966	234.024	228.218	2.032	96.202	56.506	−8.433
400	41.433	239.457	229.289	4.067	96.019	50.846	−6.640
450	42.841	244.419	230.698	6.174	95.712	45.217	−5.249
500	44.168	249.002	232.303	8.350	95.311	39.627	−4.140
600	46.530	257.270	235.790	12.888	94.307	28.581	−2.488
700	48.483	264.595	239.391	17.642	93.123	17.718	−1.322
800	50.064	271.176	242.960	22.572	91.819	7.034	−0.459
900	51.336	277.149	246.432	27.645	90.425	−3.482	0.202
1000	52.359	282.612	249.781	32.831	88.957	−13.838	0.723
1100	53.186	287.643	252.997	38.110	87.421	−24.043	1.142
1200	53.861	292.300	256.081	43.464	85.822	−34.106	1.485
1300	54.414	296.634	259.036	48.878	84.162	−44.033	1.769
1400	54.873	300.684	261.867	54.343	82.441	−53.831	2.008
1500	55.256	304.483	264.583	59.850	80.659	−63.503	2.211
1600	55.579	308.060	267.190	65.392	78.815	−73.053	2.385
1700	55.853	311.438	269.694	70.964	76.909	−82.487	2.535
1800	56.088	314.637	272.103	76.562	74.939	−91.807	2.664
1900	56.289	317.675	274.422	82.181	72.905	−101.015	2.777
2000	56.464	320.567	276.658	87.819	70.807	−110.115	2.876
2100	56.616	323.326	278.815	93.473	68.643	−119.108	2.963
2200	56.750	325.963	280.898	99.141	66.413	−127.997	3.039
2300	56.867	328.488	282.913	104.822	64.117	−136.782	3.106
2400	56.971	330.911	284.863	110.514	−38.764	−143.329	3.119
2500	57.064	333.238	286.752	116.216	−41.349	−147.633	3.085
2600	57.147	335.478	288.583	121.927	−43.937	−151.833	3.050
2700	57.220	337.636	290.360	127.645	−46.527	−155.934	3.017
2800	57.287	339.718	292.086	133.371	−49.120	−159.938	2.984
2900	57.347	341.730	293.763	139.103	−51.718	−163.851	2.951
3000	57.401	343.675	295.395	144.840	−54.319	−167.673	2.919
3100	57.451	345.558	296.983	150.583	−56.924	−171.408	2.888
3200	57.496	347.382	298.529	156.330	−59.533	−175.060	2.858
3300	57.537	349.152	300.037	162.082	−62.147	−178.630	2.827
3400	57.575	350.870	301.506	167.837	−64.765	−182.120	2.798
3500	57.609	352.540	302.941	173.597	−67.388	−185.534	2.769
3600	57.641	354.163	304.341	179.359	−70.015	−188.872	2.740
3700	57.670	355.743	305.709	185.125	−72.647	−192.138	2.712
3800	57.697	357.281	307.046	190.893	−75.283	−195.331	2.685
3900	57.722	358.780	308.354	196.664	−77.923	−198.456	2.658
4000	57.746	360.242	309.633	202.437	−80.567	−201.513	2.631
4100	57.767	361.668	310.884	208.213	−83.216	−204.504	2.605
4200	57.787	363.060	312.110	213.991	−1045.567	−193.382	2.405
4300	57.806	364.420	313.311	219.770	−1046.050	−173.086	2.103
4400	57.824	365.750	314.488	225.552	−1046.541	−152.779	1.814
4500	57.840	367.049	315.641	231.335	−1047.040	−132.461	1.538
4600	57.855	368.321	316.773	237.120	−1047.548	−112.132	1.273
4700	57.870	369.565	317.883	242.906	−1048.066	−91.791	1.020
4800	57.883	370.784	318.972	248.694	−1048.595	−71.439	0.777
4900	57.896	371.977	320.042	254.483	−1049.135	−51.076	0.544
5000	57.908	373.147	321.092	260.273	−1049.687	−30.701	0.321
5100	57.919	374.294	322.124	266.064	−1050.252	−10.316	0.106
5200	57.930	375.419	323.138	271.857	−1050.832	10.080	−0.101
5300	57.940	376.522	324.135	277.650	−1051.426	30.488	−0.300
5400	57.949	377.605	325.115	283.445	−1052.037	50.907	−0.492
5500	57.958	378.669	326.080	289.240	−1052.665	71.338	−0.678
5600	57.967	379.713	327.028	295.036	−1053.312	91.780	−0.856
5700	57.975	380.739	327.961	300.833	−1053.978	112.234	−1.029
5800	57.982	381.747	328.880	306.631	−1054.665	132.700	−1.195
5900	57.990	382.739	329.784	312.430	−1055.375	153.177	−1.356
6000	57.997	383.713	330.675	318.229	−1056.108	173.668	−1.512

PREVIOUS: June 1966 (1 atm) CURRENT. June 1966 (1 bar)

$S°(298.15 \text{ K}) = 242.60 \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = -457.3 \pm 8.4 \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = -456.1 \pm 8.4 \text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}	ν, cm^{-1}
2065(1)	565(2)
570(1)	285(2)
1910(1)	

Ground State Quantum Weight: 1
Point Group: $D_{\infty h}$ σ = 2
Bond Distances: O–B = 1.20 Å; B–B = 1.70 Å
Bond Angle: O–B–B = 180°
Rotational Constant: $B_0 = 0.112313 \text{ cm}^{-1}$

Enthalpy of Formation

$\Delta_f H°(B_2O_2$, g, 298.15 K) adopted is the weighted average of three $\Delta_f H°$(298 15 K) values derived from two different chemical reactions. The chemical reactions related to the production of B_2O_2(g) have been studied by several investigators. Using the equilibrium vapor pressure data, the respective values of $\Delta_r H°$(298 15 K) were evaluated by both the 2nd and 3rd law methods. The results obtained are based on the latter and presented as follows:

Source	Reaction	$\Delta_r H°$(298.15 K), kcal·mol^{-1} 2nd law	 3rd law	$\Delta_f H°$(298.15 K) kcal·mol^{-1}
1	2/3 B(cr) + 2/3 B_2O_3(l) = B_2O_2(g)	94.0	91.8 ± 2.2	−105.5 ± 0.7*
	2/3 B(cr) + 2/3 B_2O_3(g) = B_2O_2(g)	24.8	25.4 ± 0.2	−108.0 ± 0.5
2	2 MgO(cr) + 2 B(cr) = 2 Mg(g) + B_2O_2(g)	255.4	—	−102.6 ± 10*
3	2/3 B(cr) + 2/3 B_2O_3(l) = B_2O_2(g)	89.3	77.9 ± 0.2	−110.2 ± 0.9
4	B_2O_3(l) + 3 C(cr) = 3 CO(g) + 2 B(cr)	—	—	−108.5 ± 1.5
	B_2O_3(l) + C(cr) = B_2O_2(g) + CO(g)	—	—	

*The value not used for the calculation of the weighted average of $\Delta_f H°(B_2O_2$, g, 298.15 K).

Heat Capacity and Entropy

The molecular structure and constants, and vibrational frequencies, corrected to the average isotopic species, were taken from Sommer *et al.*[5]

References

[1] M. G. Inghram, R. F. Porter and W A. Chupka, J Chem. Phys. **25**, 498 (1956).
[2] A. W. Searcy and C. E. Myers, J. Phys. Chem. **61**, 957 (1957).
[3] M. D. Scheer, J. Phys Chem. **62**, 490 (1958).
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[5] O. Sommer, D. White, M. J. Linevsky, and D. E. Mann, J. Phys. Chem. **38**, 87 (1963).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ J·K^{-1}mol^{-1}	$S°$ J·K^{-1}mol^{-1}	$-[G°-H°(T_r)]/T$ J·K^{-1}mol^{-1}	$H°-H°(T_r)$ kJ·mol^{-1}	$\Delta_f H°$ kJ·mol^{-1}	$\Delta_f G°$ kJ·mol^{-1}	log K_f
0	0.	0.	INFINITE	−12.398	−457.343	−457.343	INFINITE
100	34.367	193.295	286.969	−9.367	−457.265	−459.202	239.863
200	48.231	221.483	247.582	−5.220	−456.694	−461.326	120.486
250	53.477	232.836	243.520	−2.671	−456.345	−462.525	96.639
298.15	57.297	242.597	242.597	0.	−456.056	−463.743	81.246
300	57.424	242.952	242.598	0.106	−456.046	−463.791	80.753
350	60.445	252.040	243.309	3.056	−455.827	−465.100	69.412
400	62.871	260.275	244.923	6.141	−455.708	−466.434	60.910
450	64.921	267.802	247.053	9.337	−455.684	−467.777	54.298
500	66.722	274.737	249.479	12.629	−455.741	−469.118	49.008
600	69.820	287.184	254.750	19.461	−456.031	−471.770	41.071
700	72.409	298.147	260.182	26.576	−456.480	−474.359	35.397
800	74.575	307.962	265.551	33.928	−457.030	−476.877	31.137
900	76.378	316.853	270.765	41.479	−457.649	−479.321	27.819
1000	77.874	324.980	275.786	49.194	−458.320	−481.694	25.161
1100	79.116	332.462	280.603	57.045	−459.038	−483.996	22.983
1200	80.149	339.392	285.217	65.010	−459.800	−486.232	21.165
1300	81.013	345.842	289.635	73.069	−460.607	−488.402	19.624
1400	81.739	351.873	293.868	81.208	−461 461	−490.509	18.301
1500	82.353	357.534	297.925	89.413	−462.365	−492.552	17.152
1600	82.876	362.866	301.819	97.675	−463.323	−494.534	16.145
1700	83.323	367.904	305.560	105.986	−464.337	−496.454	15.254
1800	83.709	372.678	309.157	114.338	−465.410	−498.313	14.461
1900	84.042	377.213	312.621	122.726	−466.544	−500.110	13.749
2000	84.333	381.532	315.959	131.145	−467.743	−501.846	13.107
2100	84.588	385.653	319.180	139.591	−469.007	−503.520	12.524
2200	84.812	389.593	322.292	148.062	−470.339	−505.132	11.993
2300	85.010	393.367	325.301	156.553	−471.740	−506.683	11.507
2400	85.185	396.989	328.213	165.063	−573.730	−506.034	11.014
2500	85.342	400.470	331.034	173.589	−575.428	−503.178	10.513
2600	85.482	403.820	333.770	182.131	−577.133	−500.254	10.050
2700	85.608	407.048	336.424	190.685	−578.846	−497.265	9.620
2800	85.722	410.164	339.002	199.252	−580.567	−494.211	9.220
2900	85.824	413.174	341.508	207.829	−582.297	−491.098	8.846
3000	85.917	416.085	343.946	216.416	−584.037	−487.923	8.495
3100	86.002	418.903	346.319	225.012	−585.787	−484.690	8.167
3200	86.079	421.635	348.630	233.617	−587.546	−481.401	7.858
3300	86.150	424.285	350.883	242.228	−589.316	−478.057	7.567
3400	86.214	426.858	353.079	250.846	−591.095	−474.658	7.292
3500	86.274	429.358	355.223	259.471	−592.885	−471.208	7.032
3600	86.328	431 789	357.317	268.101	−594.684	−467.706	6.786
3700	86.379	434.155	359.361	276.736	−596.492	−464.154	6.553
3800	86.426	436.459	361.360	285.377	−598.311	−460.552	6.331
3900	86.469	438.705	363.315	294.021	−600.138	−456.903	6.120
4000	86.509	440.894	365.227	302.670	−601.975	−453.208	5.918
4100	86.547	443.031	367.099	311.323	−603.820	−449.466	5.726
4200	86.581	445.117	368.931	319.979	−1565.374	−431.630	5.368
4300	86 614	447.155	370.727	328.639	−1565.063	−404.640	4.915
4400	86 644	449.146	372.487	337.302	−1564.766	−377.657	4.483
4500	86.672	451.094	374.212	345.968	−1564.481	−350.681	4.071
4600	86.699	452.999	375.904	354.637	−1564.211	−323 711	3.676
4700	86.724	454.864	377.564	363.308	−1563.955	−296.746	3.298
4800	86.747	456.690	379.194	371.981	−1563.715	−269.787	2.936
4900	86.769	458.479	380.794	380.657	−1563.492	−242.831	2.589
5000	86.790	460.232	382.365	389.335	−1563.287	−215.881	2.255
5100	86.810	461.951	383.909	398.015	−1563.101	−188.935	1.935
5200	86.828	463.637	385.426	406.697	−1562.935	−161.993	1.627
5300	86.846	465.291	386.917	415.381	−1562.791	−135.052	1.331
5400	86.862	466.914	388.384	424.066	−1562.670	−108.116	1.046
5500	86.878	468.508	389.826	432.753	−1562.573	−81.181	0.771
5600	86.893	470.074	391.245	441.442	−1562.503	−54.246	0.506
5700	86.907	471.612	392.641	450.132	−1562.461	−27.314	0.250
5800	86.920	473.124	394.016	458.823	−1562.449	−0.381	0.003
5900	86.933	474.609	395.370	467.516	−1562.468	26.550	−0.235
6000	86.945	476.071	396.702	476.210	−1562.521	53.484	−0.466

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Boron Oxide (B_2O_3) CRYSTAL $M_r = 69.6182$ Boron Oxide (B_2O_3) $B_2O_3(cr)$

$\Delta_f H°(0\ K) = -1265.8 \pm 2.1\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = -1271.9 \pm 2.1\ kJ·mol^{-1}$
$\Delta_{fus} H° = 24.071 \pm 0.4\ kJ·mol^{-1}$

$S°(298.15\ K) = 53.95 \pm 0.4\ J·K^{-1}·mol^{-1}$
$T_{fus} = 723 \pm 0.5\ K$

Enthalpy of Formation

The adopted $\Delta_f H°(B_2O_3$, cr, 298.15 K) = 304.0 ± 0.5 $kcal·mol^{-1}$ is calculated from JANAF $\Delta_f H°(BF_3$, g, 298.15 K) = −271.42 ± 0.4 $kcal·mol^{-1}$[1] and $\Delta_c H°$(298.15 K) = −238.82 ± 0.39 $kcal·mol^{-1}$ for $B_2O_c(cr) + 3\ F_2(g) \rightarrow 2\ BF_3(g) + 1.5\ O_2(g)$. The enthalpy of combustion of $B_2O_3(cr)$ in fluorine was determined by Johnson and Hubbard.[2] The direct combusion of boron in oxygen has led to $\Delta_f H°$(glass, 298.15 K) values which range from −280 to −368 $kcal·mol^{-1}$[3-9] due to incomplete combustions or ill-defined states of combustion products. These values are not reliable.

A reliable enthalpy of formation of boric oxide can be derived from enthalpies of solution of $H_3BO_3(cr)$ and $B_2O_3(cr)$ which are listed below. Since the enthalpies of dilution of aqueous H_3BO_3[10] are relatively small, no correction has been applied to the reported enthalpy of solution data. The derived $\Delta_f H°$ values are in very good agreement with the values adopted.

Source	Enthalpy of Solution, $kcal·mol^{-1}$ $\Delta_{sol}H°(B_2O_3, cr)^{(a)}$	$\Delta_{sol}H°(H_3BO_3, cr)^{(b)}$	$\Delta_r H°(cr)^{(c)}$ $kcal·mol^{-1}$	$\Delta_f H°(B_2O_3$, cr, 298.15 K)^d $kcal·mol^{-1}$
11	−3.56*	+5.3	−14.16	−303.83
12	−3.41*	+5.10	−13.61	−304.38
13	−3.49*	+5.3	−14.09	−303.90
14	−3.48	+5.27	−14.02	−303.97
15	−3.49	+5.17	−13.83	−304.16
16	−3.45	+5.45	−14.35	−303.64

*The enthalpy of solution of B_2O_3(am) was combined with $\Delta_r H°(25°C) = 4.44\ kcal·mol^{-1}$[2] to obtain the $\Delta_{sol}H°(B_2O_3$, cr)
(a) $B_2O_3(cr) + 3\ H_2O(l) \rightarrow 2\ H_3BO_3(aq)$ (b) $H_3BO_3(cr) \rightarrow H_3BO_3(aq)$ (c) $B_2O_3(cr) + 3\ H_2O(l) \rightarrow 2\ H_3BO_3(cr)$
(d) the auxiliary data $\Delta_f H°(H_3BO_3$, cr, 298.15 K)[1] = −261.47 ± 0.2 $kcal/mol^{-1}$ and $\Delta_f H°(H_2O$, l, 298.15 K)[10] = −68.315 $kcal\ mol^{-1}$ are used in the calculation.

Other solution calorimetric measurements[17-19] which involve the hydrolysis of $B_2H_6(g)$ and $BCl_3(l)$ lead to enthalpies of formation of boric oxide (cr) with a relatively large uncertainty since the techniques were indirect, and many questionable auxiliary data were employed in the derivation.

Heat Capacity and Entropy

The adopted heat capacities are derived from C_p data of Kerr, Hersh and Johnston[20] and Shmidt[21] in the temperature regions 18–296.6 K and 303–703 K, respectively. These two sets of C_p data were measured adiabatically and are smoothly joined at 298.15 K by a polynomial curve fitting technique. The derived entropy, $S°$(298.15 K), is based on $S°(18.08\ K) = 0.025\ cal·K^{-1}·mol^{-1}$.

Kelley[22] also measured low temperature C_p from 53 to 295 K which are in very good agreement with the values adopted. Southard[23] determined high temperature enthalpy data from 350 to 721.5 K by drop calorimetry. The deviations of the observed enthalpy data from the adopted values are about 5% at 360 K, 1% at 570 K and 0.5% at 720 K.

Fusion Data

The melting point, 723 ± 0.5 K, was determined by Schmidt[21] in excellent agreement with the value 723 ± 2 K reported by Kracek *et al.*[24] The adopted enthalpy of fusion, $\Delta_{fus}H° = 5.75 \pm 0.1\ kcal·mol^{-1}$, is derived from $\Delta_r H°(298.15\ K) = 4.44\ kcal·mol^{-1}$ for $B_2O_3(crystal) \rightarrow B_2O_3(am)$[2] and the adopted relative enthalpies of the two forms at 723 K. This value is reasonable agreement with $\Delta_{fus}H°(723\ K) = 5.87 \pm 0.1\ kcal·mol^{-1}$ determined calorimetrically by Schmidt.[21]

References

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.293	−1265.776	−1265.776	INFINITE
100	20.740	10.983	96.353	−8.537	−1269.425	−1244.466	650.042
200	43.844	32.869	59.093	−5.245	−1271.165	−1218.726	318.299
298.15	62.588	53.953	53.953	0.	−1271.936	−1192.796	208.973
300	62.927	54.341	53.954	0.116	−1271.944	−1192.305	207.599
400	77.948	74.600	56.614	7.194	−1272.047	−1165.729	152.229
500	89.287	93.269	62.105	15.582	−1271.710	−1139.180	119.009
600	98.115	110.360	68.744	24.969	−1271.024	−1112.733	96.872
700	105.228	126.039	75.825	35.149	−1270.036	−1086.426	81.070
723 000	106.692	129.464	77.477	37.587	--- CRYSTAL <--> LIQUID ---		
800	111.169	140.489	83.017	45.978	−1268.779	−1060.279	69.229
900	116.190	153.879	90.156	57.351	−1267.277	−1034.304	60.029
1000	120.625	166.356	97.159	69.197	−1265.548	−1008.509	52.679
1100	124.516	178.039	103.986	81.458	−1263.611	−982.897	46.674
1200	128.072	189.029	110.620	94.092	−1261.478	−957.470	41.678
1300	131.294	199.409	117.054	107.061	−1259.167	−932.228	37.457
1400	134.306	209.251	123.291	120.344	−1256.684	−907.171	33.847
1500	137.110	218.614	129.336	133.916	−1254.042	−882.298	30.724

PREVIOUS December 1964 CURRENT. June 1971

Boron Oxide (B_2O_3) LIQUID $M_r = 69.6182$ Boron Oxide (B_2O_3) $B_2O_3(l)$

$S°(298.15\ \mathrm{K}) = [78.443 \pm 0.4]\ \mathrm{J \cdot K^{-1} \cdot mol^{-1}}$
$T_{fus} = 723 \pm 0.5\ \mathrm{K}$

$\Delta_f H°(298.15\ \mathrm{K}) = [-1253.359 \pm 2.5]\ \mathrm{kJ \cdot mol^{-1}}$
$\Delta_{fus} H° = 24.071 \pm 0.4\ \mathrm{kJ \cdot mol^{-1}}$

Enthalpy of Formation

$\Delta_f H°$(l, 298.15 K), is calculated from $\Delta_r H°(25°\mathrm{C}) = 4.44 \pm 0.06\ \mathrm{kcal \cdot mol^{-1}}$[1] for $B_2O_3(cr) \rightarrow B_2O_3(glass)$, using the JANAF value $\Delta_f H°(B_2O_3, cr, 298.15\ \mathrm{K}) = -304.0 \pm 0.5\ \mathrm{kcal\ mol^{-1}}$. The value of $\Delta_r H°$ is the difference between the enthalpies of crystalline and glassy B_2O_3 determined by Johnson and Hubbard.[1]

Heat Capacity and Entropy

Heat capacities of B_2O_3(glass) have been measured adiabatically in the temperature regions 59 6–295 K by Turdakin and Tarasov,[2] and 306.7–910.8 K by Schmidt.[3] Thomas and Parks[4] also measured isothermally the heat capacities from 308 to 594 K in a radiation calorimeter. Both Schmidt[3] and Thomas and Parks[4] observed a rapid rise in heat capacity in the region 500–580 K. This rise indicates a glass transition in liquid B_2O_3.

Southard[5] and Krasovitskaya *et al.*[6] determined enthalpy changes by drop calorimetry in the temperature regions 381.7–1776.8 K and 1015–2154 K, respectively.

We have adopted the C_p data of Turdakın (60–295 K) and Shmıdt (307–600 K) which are smoothly joined at 298.15 K by a polynomial curve fitting technique. The drop calorimetric data of Southard in this region 381 to 600 K are less reliable since the final state of the sample was dependent upon previous thermal history through the glass transition region. Above the melting point, we have chosen a constant C_p, 31.0 $\mathrm{cal \cdot K^{-1} \cdot mol^{-1}}$, which is a compromise between the adiabatic C_p and drop calorimetric data. The uncertainty of this choice, ±0.6 $\mathrm{cal \cdot K^{-1} \cdot mol^{-1}}$, is within the experimental errors of both techniques.

$S°(298.15\ \mathrm{K})$ is calculated from that of the crystal by adding $\Delta_{fus}H°/T_{fus}$ and the difference in entropy, $S°(723\ \mathrm{K}) - S°(298.15\ \mathrm{K})$, between the crystal and liquid.

Fusion Data

Refer to the crystal table for details.

Vaporization Data

The boiling point is calculated as the temperature at which the fugacity is 1 bar for $B_2O_3(l) \rightarrow B_2O_3(g)$. The enthalpy of vaporization is the difference in $\Delta_f H°$ at the boiling point between liquid and gas.

References

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

		$\mathrm{J \cdot K^{-1} mol^{-1}}$			$\mathrm{kJ \cdot mol^{-1}}$		
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	16.617	INFINITE	−10.060	−1247.966	−1247.966	INFINITE
100	25.786	32.674	122.342	−8.967	−1251.278	−1228.488	641.696
200	45 915	56.849	83.667	−5.363	−1252.707	−1205.064	314.730
298.15	62.802	78.443	78.443	0.	−1253.359	−1181.521	206.998
300	63.095	78.832	78.444	0.116	−1253.366	−1181.075	205.644
400	77.404	98.998	81.097	7.160	−1253.504	−1156.945	151.082
500	89.203	117.606	86.563	15.522	−1253.193	−1132.832	118.346
600	132.842	138.348	93.368	26.988	−1250.428	−1108.930	96.541
700	129.788	158.562	101.280	40.097	−1246.511	−1085.668	81.014
723 000	129.704	162.757	103.170	43.081	--- CRYSTAL <--> LIQUID ---		
800	129.704	175.883	109.547	53.069	−1243.111	−1062.926	69.402
900	129.704	191.160	117.783	66.039	−1240.012	−1040.592	60.394
1000	129.704	204.826	125.816	79.009	−1237.159	−1018.589	53.206
1100	129.704	217.188	133.570	91.980	−1234.512	−996.861	47.337
1200	129.704	228.474	141.015	104.950	−1232.043	−975.367	42.457
1300	129.704	238.855	148.147	117.921	−1229.730	−954.072	38.335
1400	129.704	248.468	154.974	130.891	−1227.560	−932.950	34.809
1500	129.704	257.416	161.509	143.861	−1225.520	−911.979	31.758
1600	129.704	265.787	167.767	156.832	−1223.603	−891.139	29.093
1700	129.704	273.650	173.767	169.802	−1221.802	−870.416	26.745
1800	129.704	281.064	179.524	182.773	−1220.115	−849.796	24.660
1900	129.704	288.077	185.054	195.743	−1218.537	−829.266	22.798
2000	129.704	294.730	190.373	208.713	−1217.065	−808.817	21.124
2100	129.704	301.058	195.494	221.684	−1215.698	−788.438	19.611
2200	129.704	307.092	200.431	234.654	−1214.434	−768.122	18.238
2300	129.704	312.857	205.195	247.625	−1213.271	−747.862	16.984
2400	129.704	318.378	209.796	260.595	−1312.727	−725.513	15.790
2500	129.704	323.672	214.246	273.565	−1311.919	−701.062	14.648
2600	129.704	328.759	218.553	286.536	−1311.143	−676.643	13.594
2700	129.704	333.654	222.726	299.506	−1310.398	−652.253	12.619
2800	129.704	338.371	226.773	312.477	−1309.685	−627.890	11.713
2900	129.704	342.923	230.700	325.447	−1309.001	−603.554	10.871
3000	129.704	347.320	234.514	338.417	−1308.346	−579.238	10.085

PREVIOUS: December 1964   CURRENT: June 1971

Boron Oxide (B_2O_3) $B_2O_3(l)$

Boron Oxide (B_2O_3) CRYSTAL-LIQUID

0 to 723 K crystal
above 723 K liquid

Refer to the individual tables for details.

$M_r = 69.6182$ Boron Oxide (B_2O_3) $B_2O_3(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−9.293	−1265.776	−1265.776	INFINITE
100	20.740	10.983	96.353	−8.537	−1269.425	−1244 466	650.042
200	43.844	32.869	59.093	−5.245	−1271.165	−1218.726	318.299
298.15	62.588	53.953	53.953	0.	−1271.936	−1192.796	208.973
300	62.927	54.341	53.954	0.116	−1271.944	−1192.305	207.599
400	77.948	74 600	56.614	7.194	−1272.047	−1165.729	152.229
500	89.287	93.269	62.105	15.582	−1271.710	−1139.180	119.009
600	98.115	110.360	68.744	24.969	−1271.024	−1112.733	96.872
700	105.228	126.039	75.825	35.149	−1270.036	−1086.426	81.070
723.000	106.692	129.464	77.477	37.587	CRYSTAL <--> LIQUID	TRANSITION	
723.000	129.704	162.757	77.477	61.657			
800	129.704	175.883	86.328	71.644	−1243.112	−1062.927	69.402
900	129.704	191.160	97.144	84.615	−1240.014	−1040.593	60.394
1000	129.704	204.826	107.241	97.585	−1237.160	−1018.590	53.206
1100	129.704	217.188	116.683	110.556	−1234.514	−996.863	47.337
1200	129.704	228.474	125.535	123.526	−1232.044	−975.368	42.457
1300	129.704	238.855	133.858	136.496	−1229.732	−954.074	38.335
1400	129.704	248.468	141.706	149.467	−1227.561	−932.951	34.809
1500	129.704	257.416	149.125	162.437	−1225.521	−911.980	31.758
1600	129.704	265.787	156.157	175.408	−1223.604	−891.141	29.093
1700	129.704	273.650	162.840	188.378	−1221.804	−870.417	26.745
1800	129.704	281.064	169.204	201.348	−1220.116	−849.797	24.660
1900	129.704	288.077	175.277	214.319	−1218.538	−829.267	22.798
2000	129.704	294.730	181.085	227.289	−1217.066	−808.818	21.124
2100	129.704	301.058	186.649	240.260	−1215.699	−788.439	19.611
2200	129.704	307.092	191.987	253.230	−1214.435	−768.123	18.238
2300	129.704	312.857	197.118	266.200	−1213.272	−747.863	16.985
2400	129.704	318.378	202.056	279.171	−1312.728	−725.514	15.790
2500	129.704	323.672	206.816	292.141	−1311.920	−701.063	14.648
2600	129.704	328.759	211.409	305.112	−1311.144	−676.644	13.594
2700	129.704	333.654	215.846	318.082	−1310.400	−652.254	12.619
2800	129.704	338.372	220.139	331.052	−1309.686	−627.891	11.713
2900	129.704	342.923	224.294	344.023	−1309.002	−603.555	10.871
3000	129.704	347.320	228.322	356.993	−1308.347	−579.240	10.085

PREVIOUS: CURRENT June 1971

Boron Oxide (B_2O_3) $B_2O_3(cr,l)$

Boron Oxide (B_2O_3) IDEAL GAS $M_r = 69.6182$ Boron Oxide (B_2O_3) $B_2O_3(g)$

$S^\circ(298.15\ K) = [283.8 \pm 4.2]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH^\circ(0\ K) = -834.8 \pm 4.2\ kJ{\cdot}mol^{-1}$
$\Delta_fH^\circ(298.15\ K) = -836.0 \pm 4.2\ kJ{\cdot}mol^{-1}$

				Vibrational Frequencies (all single degenerate)				
υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}	υ,cm^{-1}	ν, cm^{-1}
2073	730	521	[172]	[460]	2073	1240	457	480

Ground State Quantum Weight: 1 $\sigma = 2$
Point Group: C_{2v}
Bond Distances: O–B = 1.36 ± 0.02 Å; B–O = 1.20 ± 0 03 Å
Bond Angles: O–B–O = 180°; B–O–B = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = 3.153764 \times 10^{-114}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The vapor pressure of $B_2O_3(l)$ was measured by many investigators using various methods. 2nd and 3rd law analyses of these data[1-11] are given below. We have adopted the 3rd law enthalpy of vaporization, $\Delta_{vap}H^\circ(298.15\ K) = 99\ 75\ kcal{\cdot}mol^{-1}$, to derive $\Delta_fH^\circ(B_2O_3, g, 298.15\ K) = -199.8 \pm 1\ kcal{\cdot}mol^{-1}$, using $\Delta_fH^\circ(B_2O_3, l, 298.15\ K) = -299.56\ kcal\ mol^{-1}$. The adopted $\Delta_{vap}H^\circ(298.15\ K)$ is calculated from Hildenbrand's data[1] and this value also serves as an average of all derived enthalpies of vaporization except that of Cole.[11] The uncertainty is assigned to be at least ±1 kcal·mol^{-1} since the bending frequency was estimated to be either 172 or 260 cm^{-1} [12] which could lead to a difference ±1 kcal·mol^{-1} in the $\Delta_{vap}H^\circ$ calculation through the Gibbs energy functions of $B_2O_3(g)$.

Source	T/K	Method	Data Points	$\Delta_{vap}H^\circ(298.15\ K)$, kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_fH^\circ(298.15\ K)$ kcal·mol^{-1}
1	1436–1584	Torsion–effusion	24	100.97 ± 1.34	99.75 ± 0.35	−0.8 ± 0.7	−199.81
2	1946–2419	Transpiration and direct boiling point	16	92.55 ± 2.52	102.80 ± 1.8	4.6 ± 1.2	−196.76
3	1300	Mass spectrometric	—	100.5 ± 3	—	—	−199.06
4	1325–1547	Knudsen–effusion	9	93.08 ± 1.37	99.08 ± 0.74	4.2 ± 1.0	−200.48
5	1228l–1641	Mass spectrometric	16	92.32 ± 0.94	99.17 ± 1.40	4.6 ± 0.6	−200.39
6	1229–1515	Knudsen–effusion	12	82.65 ± 2.85	98.52 ± 1.70	11.1 ± 2.0	−201.04
7	1414–1621	Torsion–effusion	19	95.55 ± 0.91	101.50 ± 0.56	3.80 ± 0.62	−198.06
8	1501–1566	Effusion	6	101.67 ± 12.46	98.31 ± 0.79	−2.2 ± 8.1	−201.25
9	1567–1808	Carrier gas	6	66.17 ± 7.8	98.00 ± 5.06	18.8 ± 4.9	−201.56
10	1331–1642	Knudsen effusion	22[a]	89.64 ± 1.62	99.06 ± 1.44	6.4 ± 1.1	−200.50
11	1473–1673	Carrier gas	6	73.27 ± 2.28	87.36 ± 1.48	9.0 ± 1.4	−212.20

[a] Four points were rejected due to failure of a statistical test.

Heat Capacity and Entropy

The V shaped molecular structure for B_2O_3 was proposed by many investigators on the basis of infrared spectrometry[12,13] and electron diffraction.[14] This structure has been reconfirmed by recent electric deflection[15] and electron diffraction[16] studies which definitely rule out any non polar structure such as the bipyramidal model as suggested by Hanst *et al.*[17] Thus the assignment of vibrational frequencies, based on the V shaped structure, should be valid. The adopted vibrational frequencies (including two estimated values) were obtained from Sommer *et al.*[12] in their infrared spectrometric studies. Their values have been adjusted to the average isotopic species. Other spectrometric data[13,18] are in reasonable agreement with those adopted in the tabulation.

Akishin and Spiridonov[14] determined the bond distances and bond angle (B–O–B = 95°) by electron diffraction. We have adopted their bond distances in the tabulation, but tentatively select an apex angle B–O–B = 120° based on force constant calculations of Weltner and Warn[13] and Sommer *et al.*[12] The principal moments of inertia are $I_A = 2.9763 \times 10^{-39}$, $I_B = 31.0977 \times 10^{-39}$ and $I_C = 34.0740 \times 10^{-39}\ g{\cdot}cm^2$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0	0.	0.	INFINITE	−14.337	−834.847	−834.847	INFINITE
100	40.042	226.986	334.961	−10.797	−835.713	−832.354	434.777
200	55.330	259.361	289.548	−6.037	−835.985	−828.844	216.472
250	61.832	272.432	284.842	−3.102	−835.979	−827.059	172.805
298.15	66.855	283.768	283.768	0.	−835.963	−825.343	144.597
300	67.028	284.182	283 769	0.124	−835.963	−825.277	143.694
350	71.228	294.841	284 601	3.584	−835.972	−823.496	122.900
400	74.727	304.587	286.499	7.235	−836.033	−821.710	107.304
450	77.728	313.566	289.014	11.048	−836.152	−819.913	95.173
500	80.362	321.894	291.891	15.002	−836.317	−818.100	85.466
600	84.817	336.954	298.173	23.269	−836.752	−814.418	70.901
700	88.439	350.310	304.685	31.938	−837.275	−810.655	60 492
800	91.403	362.320	311.151	40.935	−837.849	−806.814	52.680
900	93.830	373.230	317.452	50.200	−838.455	−802.898	46.599
1000	95.822	383.223	323.537	59.686	−839.087	−798.914	41.731
1100	97 462	392.435	329.387	69.353	−839.743	−794.864	37.745
1200	98.819	400.975	335.001	79.169	−840.428	−790.755	34.421
1300	99.950	408.931	340.386	89.109	−841.146	−786.586	31.605
1400	100.897	416.374	345.550	99.153	−841.902	−782.361	29.190
1500	101.696	423.363	350.507	109.284	−842.701	−778.081	27.095
1600	102.375	429.949	355.269	119.488	−843.550	−773.746	25.260
1700	102.955	436.173	359.846	129.755	−844.453	−769.355	23.639
1800	103.454	442.072	364.252	140.076	−845.415	−764.911	22.197
1900	103.886	447.677	368.496	150.444	−846.440	−760.411	20.905
2000	104.262	453.016	372.590	160.852	−847.531	−755.855	19.741
2100	104.591	458.111	376.542	171.295	−848.691	−751.243	18.686
2200	104.880	462.983	380.361	181.769	−849.924	−746.573	17.726
2300	105.136	467.651	384.056	192.270	−851.230	−741.847	16.848
2400	105.363	472.131	387 633	202.795	−953.131	−734.924	15.995
2500	105.565	476.436	391.099	213.342	−954.747	−725.799	15.165
2600	105.746	480.580	394.462	223.907	−956.376	−716.609	14.397
2700	105.908	484.574	397.726	234.490	−958.019	−707.356	13.685
2800	106.054	488.428	400.897	245.088	−959.677	−698.041	13.022
2900	106.186	492.152	403.980	255.700	−961.351	−688.669	12.404
3000	106.306	495.754	406.979	266.325	−963.042	−679.237	11.827
3100	106.415	499.242	409.899	276.961	−964 749	−669.748	11.285
3200	106.515	502.622	412.744	287.608	−966.474	−660.205	10.777
3300	106.606	505.901	415.518	298.264	−968.214	−650.608	10.298
3400	106.689	509.085	418.223	308.929	−969.971	−640.956	9.847
3500	106.765	512.178	420.864	319.602	−971.744	−631.254	9 421
3600	106.836	515.187	423.442	330.282	−973.532	−621.500	9.018
3700	106.901	518.115	425.961	340.969	−975.337	−611.697	8.636
3800	106.961	520.967	428.424	351.662	−977.156	−601.843	8.273
3900	107.017	523.746	430.833	362.361	−978.991	−591.943	7.928
4000	107.069	526.456	433.190	373.065	−980.840	−581.996	7.600
4100	107.117	529 100	435.497	383.774	−982.703	−572.001	7.287
4200	107.161	531.682	437.756	394.488	−1944.280	−547.913	6.814
4300	107.203	534.204	439.970	405.206	−1943.998	−514.669	6.252
4400	107.242	536.669	442.140	415.929	−1943.734	−481.433	5.715
4500	107.279	539.080	444.267	426.655	−1943.488	−448.202	5.203
4600	107.313	541.438	446.354	437.384	−1943.261	−414.977	4.712
4700	107.345	543.746	448.402	448.117	−1943.055	−381 755	4.243
4800	107.375	546.006	450.412	458.853	−1942.871	−348.538	3.793
4900	107.403	548.221	452.386	469.592	−1942.709	−315.323	3.361
5000	107.430	550.391	454.324	480.334	−1942.570	−282.113	2.947
5100	107.455	552.518	456.229	491.078	−1942.457	−248.904	2.549
5200	107.479	554.605	458.101	501.825	−1942.370	−215.700	2.167
5300	107.502	556.653	459.941	512.574	−1942.312	−182.494	1.799
5400	107.523	558.662	461.750	523.325	−1942.285	−149.291	1.444
5500	107.543	560.636	463.530	534.078	−1942.289	−116.088	1.103
5600	107.562	562.574	465.282	544.834	−1942.328	−82.883	0.773
5700	107.580	564.477	467.005	555.591	−1942.403	−49.678	0.455
5800	107.597	566.349	468.702	566.350	−1942.517	−16.470	0.148
5900	107.613	568.188	470.373	577.110	−1942.672	16.736	−0.148
6000	107.629	569.997	472.018	587.872	−1942.870	49.949	−0.435

PREVIOUS: June 1971 (1 atm) CURRENT: June 1971 (1 bar)

Lead Borate (PbB_2O_4) CRYSTAL $M_r = 292.8176$ Lead Borate (PbB_2O_4) $B_2O_4Pb_1(cr)$

$S°(298.15\ K) = [130.5 \pm 12]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = $ Unknown
$\Delta_f H°(298.15\ K) = -1556 \pm 6\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

Evans[1] analyzed the enthalpies of formation of the lead borate system. Shartsis and Newman measured enthalpies of solution of the lead borate glasses in 2 N HNO_3. In their phase studies, Mazzetti and De Carli[3] established that the compounds formed were $PbO{\cdot}B_2O_3$, $PbO{\cdot}2B_2O_3$ and $2PbO{\cdot}5B_2O_3$. From the Shartsis and Newman[2] paper, Evans[1] obtained the following:

$$PbO(cr + B_2O_3(cr) \rightarrow PbOB_2O_3(gls) \qquad \Delta_r H° = -16.2\ kcal{\cdot}mol^{-1}$$

and estimated a $\Delta_f H°(298.15\ K)$ of 7.0 $kcal{\cdot}mol^{-1}$ for the conversion to the $PbOB_2O_3(cr)$ With auxiliary JANAF values, the $\Delta_f H°(298.15\ K)$ was calculated to be $-372\ kcal{\cdot}mol^{-1}$. The results of Lepinskikh and Esin[4] studying the lead borate system at 1000 K with cells of the type $Pb(l)/PbO,B_2O_3/Pt/O_2(g)$ were in fair agreement with the results of Shartsis and Newman.[2]

Heat Capacity and Entropy

The heat capacity employed in this table was obtained by graphically smoothing the summation of the heat capacities for $B_2O_3$and PbO.

The entropy at 298.15 was obtained from a consideration of the entropies of sodium and calcium borates and those of the constituent oxides, as given by Kelley and King.[5] These indicate for the reaction $MO + B_2O_3 \rightarrow MoB_2O_3$ that the simple addition of entropies will give values at least 2.7 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$ too low for the reaction. The reason for this is probably structural, the $B_2O_4^{--}$ ion is a flexible chain. Therefore, $S°(PbB_2O_4,\ cr,\ 298.15\ K)$ was obtained from the summation of $S°(298.15\ K)$ for constituent oxides and the addition of 2.7 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	107.110	130.541	130.541	0.	−1556.448	−1450.245	254.077
300	107.529	131.205	130.543	0.199	−1556.450	−1449.586	252.395
400	129.704	165.276	135.038	12.095	−1555.950	−1414.009	184.651
500	147.695	196.213	144.227	25.993	−1554.445	−1378.679	144.030
600	162.339	224.474	155.281	41.516	−1552.093	−1343.734	116.982
700	174.473	250.436	167.046	58.374	−1553.877	−1308.443	97.637
800	184.514	274.413	178.987	76.340	−1550.166	−1273.627	83.159
900	192.464	296.613	190.839	95.196	−1545.870	−1239.312	71.928
1000	199.577	317.281	202.462	114.819	−1541.050	−1205.503	62.969
1100	204.179	336.522	213.785	135.011	−1535.862	−1172.197	55.663
1200	208.363	354.479	224.770	155.652	−1530.390	−1139.376	49.596
1300	210.874	371.262	235.400	176.620	−1524.741	−1107.020	44.481
1400	212.547	386.945	245.671	197.784	−1519.046	−1075.101	40.113
1500	215.058	401.700	255.586	219.172	−1513.274	−1043.592	36.341
1600	216.731	415.631	265.157	240.758	−1507.448	−1012.470	33.054
1700	218.823	428.833	274.400	262.535	−1501.572	−981.713	30.164
1800	220.915	441.402	283.332	284.526	−1495.624	−951.305	27.606
1900	222.589	453.391	291.969	306.701	−1489.630	−921.228	25.326
2000	224.262	464.851	300.329	329.044	−1483.608	−891.468	23.283

PREVIOUS December 1962 CURRENT: March 1965

Lead Borate (PbB_2O_4) $B_2O_4Pb_1(cr)$

Titanium Boride (TiB_2) **CRYSTAL** **M_r = 69.50** **Titanium Boride (TiB_2)** **$B_2Ti_1(cr)$**

$S°(298.15 K) = 28.48 \pm 0.4 J·K^{-1}·mol^{-1}$
$T_{fus} = 3193 K$

$\Delta_f H°(0 K) = -277.8 \pm 16.7 kJ·mol^{-1}$
$\Delta_f H°(298.15 K) = -279.5 \pm 16.7 kJ·mol^{-1}$
$\Delta_{fus}H° = [100.4] kJ·mol^{-1}$

Enthalpy of Formation

Kibler *et al.*[1] studied the vapor pressure of the reaction $TiB_2(cr) + 1/2 C(cr) = Ti(g) + 1/2 B_4C(cr)$ by comparing the absorption intensity of the 3371.45 Å Ti resonance line of the above reaction at temperature T_1 to Ti(g) over pure titanium metal at temperature T_2. Using JANAF auxiliary data, $\Delta G°(2475 K) = 81.612 kcal·mol^{-1}$ for the above reaction and $\Delta_f H°(TiB_2, cr, 298.15 K) = -66.9 kcal·mol^{-1}$ were calculated.

Williams[2] found 2150 ± 25 K to be the temperature at which $TiB_2(cr)$ was formed from a mixture of TiN(cr) and BN(cr). If $\Delta G°(2150 K) = 0$ is assumed for the reaction $TiN(cr) + 2 BN(cr) = TiB_2(cr) + 3/2 N_2(g)$, then $\Delta_f H°(TiB_2, cr, 298.15 K) = -70.7 kcal·mol^{-1}$. If, however, $N_2(g)$ is 1/2 atm, then $\Delta G°(2150 K) = 4.4 kcal·mol^{-1}$ and $\Delta_f H°(TiB_2, cr, 298.15 K) = -66.3 kcal·mol^{-1}$. He has also shown by stability comparisons that ΔG and $\Delta H > 0$ for the reaction $TiB_2 + 3/2 C = TiC + 1/2 B_4C$. Thus $\Delta_f H°(TiB_2, 298.15 K) < -51 kcal·mol^{-1}$.

Schissel and Trulson[3] used a mass spectrometer with Knudsen cells to study the vaporization of the titanium–boron system. Only the set of measurements without excess boron or titanium was used. The value $\Delta G°(2261 K) = 194.9 kcal·mol^{-1}$ for the reaction $TiB_2(cr) = Ti(g) + 2 B(g)$ was obtained. This corresponds to $\Delta_f H°(TiB_2, cr, 298.15 K) = -62.9 kcal·mol^{-1}$ using JANAF auxiliary data.

Epel'baum and M. I. Starostina[4] report $\Delta_f H°(TiB_2, cr, 298.15 K) = -66.85 \pm 2.7 kcal·mol^{-1}$ from combustion calorimetry.

Lowell and Williams[5] used high temperature calorimetry to obtain the enthalpy of formation of $TiB_2(cr)$. From their data and JANAF auxiliary data, $\Delta_f H°(TiB_2, cr, 298.15 K) = -48.2 \pm 5 kcal·mol^{-1}$ was calculated. We question the authenticity of the experiment and believe their value is an upper limit.

$\Delta_f H°(TiB_2, cr, 298.15 K) = -66.8 \pm 4 kcal·mol^{-1}$ was chosen as representative of the first four investigations.

Heat Capacity and Entropy

The heat capacity of $TiB_2(cr)$ has been determined by the following investigators.

Source	Method	T/K
6	Adiabatic Calorimetry	5–350
7	Drop calorimeter	373–977
8	Drop type ice calorimeter	586–2689
9	Copper–block drop calorimeter	420–1180
10	Arc–imaging furnace	1300–2150
11	Pulse–method	1733–2417

The low temperature data of Westrum[1] and the medium range data of Walker *et al.*[7] were used to obtain the C_p's of this tabulation. Their data were fitted to a Shomate plot and extrapolated to 4000 K.

$S°(298.15 K) = 6.808 cal·K^{-1}·mol^{-1}$ was determined by Westrum.[1]

Fusion Data

The melting point has been reported as 3063 K, 3193 K, and 3203 K by Glaser,[12] Post *et al.*,[13] and Samsonov and Petrash,[14] respectively. The enthalpy of fusion is derived from an estimated $\Delta_{fus}S = 2.5 cal·K^{-1} g atom^{-1}$ at 3193 K. It should be pointed out that an error of 0.5 $cal·K^{-1}·mol^{-1} g atom^{-1}$ in the estimation of $\Delta_{fus}S°$ is 5 $kcal·mol^{-1}$ in $\Delta_{fus}H°$.

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Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−5.577	−277.811	−277.811	INFINITE
100	7.523	2.518	56.366	−5.385	−278.227	−277.591	144.999
200	28.125	14.046	32.058	−3.602	−279.027	−276.623	72.247
298.15	44.279	28.485	28.485	0.	−279.491	−275.334	48.237
300	44.522	28.759	28.486	0.082	−279.498	−275.308	47 935
400	54.890	43.136	30.375	5.104	−279.814	−273.864	35.763
500	61 668	56.156	34.253	10.952	−280.169	−272.336	28.451
600	66.166	67.815	38.893	17.353	−280.556	−270.734	23.569
700	69.496	78.274	43.785	24.142	−280.964	−269.064	20 078
800	72.069	87.723	48.696	31.222	−281.376	−267.336	17.455
900	74.534	96.355	53.519	38.553	−281.799	−265.556	15.412
1000	76.889	104.331	58.206	46.125	−282.273	−263.727	13.776
1100	79.136	111.765	62.741	53.927	−282.845	−261.846	12.434
1200	81.283	118.744	67.120	61.949	−287.496	−259.788	11.308
1300	83.320	125.331	71.347	70.180	−287.529	−257.477	10.346
1400	85.249	131.577	75.428	78 609	−287.537	−255.165	9.520
1500	87.069	137.521	79.371	87.226	−287.539	−252.853	8.805
1600	88.780	143.196	83.184	96.019	−287.553	−250.540	8.179
1700	90.383	148.627	86.875	104.978	−287.599	−248.225	7.627
1800	91.876	153.836	90.451	114.092	−287.698	−245.907	7.136
1900	93.261	158 841	93.920	123.350	−287.872	−243.581	6.696
2000	94.537	163.657	97.287	132.741	−302.828	−240.789	6.289
2100	95.705	168.298	100.558	142.254	−303.964	−237.659	5.911
2200	96.763	172.775	103.740	151.878	−305.057	−234.476	5.567
2300	97.713	177.098	106.836	161.603	−306.118	−231.244	5.252
2400	98.554	181.275	109.851	171.416	−407.675	−225.829	4.915
2500	99.391	185.315	112.789	181.314	−408.851	−218.227	4.560
2600	100.228	189.229	115.654	191.295	−409.944	−210.581	4.231
2700	101.065	193.028	118.450	201.359	−410.953	−202.893	3.925
2800	101.901	196.718	121.180	211.507	−411.879	−195.170	3.641
2900	102.738	200.309	123.847	221.739	−412.721	−187.415	3.376
3000	103.575	203.806	126.454	232.055	−413.479	−179.633	3.128
3100	104 412	207.215	129.004	242.454	−414.153	−171.827	2.895
3193.000	105.190	210.313	131.328	252.201	--- CRYSTAL <--> LIQUID ---		
3200	105.249	210.544	131.501	252.937	−414.744	−164.000	2.677
3300	106 085	213.795	133.945	263.504	−415.251	−156.157	2.472
3400	106.922	216.975	136.341	274.154	−415.674	−148.299	2.278
3500	107.759	220 086	138.689	284.889	−416 014	−140.429	2.096
3600	108.596	223.133	140.993	295.706	−416.270	−132.552	1.923
3700	109.433	226.120	143.253	306 608	−825.541	−116.880	1.650
3800	110.269	229 050	145.473	317.593	−824.395	−97.742	1.344
3900	111.106	231.925	147.653	328.662	−823.221	−78.635	1.053
4000	111.943	234.748	149.795	339.814	−822.017	−59.558	0.778

PREVIOUS: December 1962 CURRENT: June 1965

Titanium Boride (TiB_2) LIQUID $M_r = 69.50$ Titanium Boride (TiB_2) $B_2Ti_1(l)$

$S°(298.15\ K) = [56.365]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 3193\ K$
$T_{dcm} = [4250]\ K$

$\Delta_f H°(298.15\ K) = [-188.029]\ kJ{\cdot}mol^{-1}$
$\Delta_{fus}H° = [100.4]\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(TiB_2, l, 298.15\ K)$ is calculated from $\Delta_f H°(TiB_2, cr, 298.15\ K)$ by adding the enthalpy of fusion, $\Delta_{fus}H°$, and the difference in enthalpy, $H°(3193\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 2100 K. Heat capacities at and below 2100 K are assumed to be equal to those of $TiB_2(cr)$. Above 2100 K the heat capacities are estimated to be constant.

$S°(TiB_2, l, 298.15\ K)$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Decomposition Data

T_{dcm} is estimated as the temperature for which $\Delta_f G° = 0$ for the reaction $TiB_2(l) \rightarrow Ti(g) + 2\ B(g)$.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0							
100							
200							
298.15	44.279	56.365	56.365	0.	−188.029	−192.185	33.670
300	44.522	56.640	56.366	0.082	−188.036	−192.211	33.467
400	54.890	71.016	58.256	5.104	−188.352	−193.554	25.276
500	61.668	84.036	62.133	10.952	−188.707	−194.814	20.352
600	66.166	95.695	66.773	17.353	−189.094	−196.000	17.063
700	69.496	106.154	71.665	24.142	−189.502	−197.119	14.709
800	72.069	115.603	76.576	31.222	−189.914	−198.179	12.940
900	74.534	124.235	81.399	38.553	−190.337	−199.187	11.560
1000	76.889	132.211	86.086	46.125	−190.811	−200.145	10.455
1100	79.136	139.646	90.621	53.927	−191.383	−201.052	9.547
1200	81.283	146.624	95.000	61.949	−196.034	−201.782	8.783
1300	83.320	153.211	99.227	70.180	−196.067	−202.260	8.127
1400	85.249	159.457	103.308	78.609	−196.075	−202.736	7.564
1500	87.069	165.402	107.251	87.226	−196.077	−203.211	7.076
1600	88.780	171.076	111.064	96.019	−196.091	−203.687	6.650
1700	90.383	176.507	114.755	104.978	−196.137	−204.160	6.273
1800	91.876	181.716	118.331	114.092	−196.236	−204.629	5.938
1900	93.261	186.721	121.800	123.350	−196.409	−205.091	5.638
2000	94.537	191.538	125.167	132.741	−211.366	−205.088	5.356
2100	95.705	196.179	128.439	142.254	−212.502	−204.746	5.093
2100.000	95.705	196.179	128.439	142.254	GLASS <--> LIQUID		
2100.000	108.784	196.179	128.439	142.254	TRANSITION		
2200	108.784	201.240	131.634	153.132	−212.341	−204.381	4.853
2300	108.784	206.075	134.766	164.011	−212.248	−204.022	4.633
2400	108.784	210.705	137.835	174.889	−312.740	−201.527	4.386
2500	108.784	215.146	140.839	185.768	−312.935	−196.889	4.114
2600	108.784	219.412	143.779	196.646	−313.131	−192.243	3.862
2700	108.784	223.518	146.657	207.524	−313.326	−187.590	3.629
2800	108.784	227.474	149.473	218.403	−313.521	−182.930	3.413
2900	108.784	231.292	152.229	229.281	−313.717	−178.262	3.211
3000	108.784	234.979	154.926	240.160	−313.912	−173.588	3.022
3100	108.784	238.546	157.567	251.038	−314.107	−168.907	2.846
3193.000	108.784	241.762	159.972	261.155	--- CRYSTAL <--> LIQUID ---		
3200	108.784	242.000	160.151	261.916	−314.303	−164.220	2.681
3300	108.784	245.348	162.683	272.795	−314.498	−159.527	2.525
3400	108.784	248.595	165.162	283.673	−314.693	−154.828	2.379
3500	108.784	251.749	167.591	294.552	−314.889	−150.124	2.240
3600	108.784	254.813	169.971	305.430	−315.084	−145.413	2.110
3700	108.784	257.794	172.305	316.308	−724.378	−132.909	1.876
3800	108.784	260.695	174.593	327.187	−723.339	−116.937	1.607
3900	108.784	263.521	176.837	338.065	−722.355	−100.992	1.353
4000	108.784	266.275	179.039	348.944	−721.426	−85.072	1.111
4100	108.784	268.961	181.199	359.822	−720.549	−69.174	0.881
4200	108.784	271.582	183.320	370.700	−1679.422	−39.249	0.488
4300	108.784	274.142	185.403	381.579	−1676.470	−0.232	0.003
4400	108.784	276.643	187.448	392.457	−1673.570	38.717	−0.460
4500	108.784	279.088	189.457	403.336	−1670.720	77.600	−0.901
4600	108.784	281.479	191.432	414.214	−1667.918	116.421	−1.322
4700	108.784	283.818	193.373	425.092	−1665.163	155.181	−1.725
4800	108.784	286.108	195.281	435.971	−1662.453	193.883	−2.110
4900	108.784	288.351	197.158	446.849	−1659.788	232.529	−2.479
5000	108.784	290.549	199.004	457.728	−1657.165	271.121	−2.832
5100	108.784	292.703	200.820	468.606	−1654.583	309.661	−3.172
5200	108.784	294.816	202.607	479.484	−1652.041	348.151	−3.497
5300	108.784	296.888	204.367	490.363	−1649.538	386.592	−3.810
5400	108.784	298.921	206.099	501.241	−1647.072	424.986	−4.111
5500	108.784	300.917	207.805	512.120	−1644.642	463.335	−4.400
5600	108.784	302.877	209.485	522.998	−1642.247	501.640	−4.679
5700	108.784	304.803	211.140	533.876	−1639.886	539.903	−4.948
5800	108.784	306.695	212.772	544.755	−1637.558	578.125	−5.207
5900	108.784	308.554	214.379	555.633	−1635.262	616.306	−5.456
6000	108.784	310.383	215.964	566.512	−1632.997	654.449	−5.697

PREVIOUS. December 1962 CURRENT: June 1965

Titanium Boride (TiB_2) CRYSTAL-LIQUID

0	to 3193 K	crystal
above	3193 K	liquid

Refer to the individual tables for details.

$M_r = 69.50$ Titanium Boride (TiB_2) $B_2Ti_1(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_fH°$ (kJ·mol⁻¹)	$\Delta_fG°$ (kJ·mol⁻¹)	log K_f
0	0.	0.	INFINITE	−5.577	−277.811	−277.811	INFINITE
100	7.523	2.518	56.366	−5.385	−278.227	−277.591	144.999
200	28.125	14.046	32.058	−3.602	−279.027	−276.623	72.247
298.15	44.279	28.485	28.485	0.	−279.491	−275.334	48.237
300	44.522	28.759	28.486	0.082	−279.498	−275.308	47.935
400	54.890	43.136	30.375	5.104	−279.814	−273.864	35.763
500	61.668	56.156	34.253	10.952	−280.169	−272.336	28.451
600	66.166	67.815	38.893	17.353	−280.556	−270.734	23.569
700	69.496	78.274	43.785	24.142	−280.964	−269.064	20.078
800	72.069	87.723	48.696	31.222	−281.376	−267.336	17.455
900	74.534	96.355	53.519	38.553	−281.799	−265.556	15.412
1000	76.889	104.331	58.206	46.125	−282.273	−263.727	13.776
1100	79.136	111.765	62.741	53.927	−282.845	−261.846	12.434
1200	81.283	118.744	67.120	61.949	−287.496	−259.788	11.308
1300	83.320	125.331	71.347	70.180	−287.529	−257.477	10.346
1400	85.249	131.577	75.428	78.609	−287.537	−255.165	9.520
1500	87.069	137.521	79.371	87.226	−287.539	−252.853	8.805
1600	88.780	143.196	83.184	96.019	−287.553	−250.540	8.179
1700	90.383	148.627	86.875	104.978	−287.599	−248.225	7.627
1800	91.876	153.836	90.451	114.092	−287.698	−245.907	7.136
1900	93.261	158.841	93.920	123.350	−287.872	−243.581	6.696
2000	94.537	163.657	97.287	132.741	−302.828	−240.789	6.289
2100	95.705	168.298	100.558	142.254	−303.964	−237.659	5.911
2200	96.763	172.775	103.740	151.878	−305.057	−234.476	5.567
2300	97.713	177.098	106.836	161.603	−306.118	−231.244	5.252
2400	98.554	181.275	109.851	171.416	−407.675	−225.829	4.915
2500	99.391	185.315	112.789	181.314	−408.851	−218.227	4.560
2600	100.228	189.229	115.654	191.295	−409.944	−210.581	4.231
2700	101.065	193.028	118.450	201.359	−410.953	−202.893	3.925
2800	101.901	196 718	121.180	211.507	−411.879	−195.170	3.641
2900	102.738	200.309	123.847	221.739	−412.721	−187.415	3.376
3000	103.575	203.806	126.454	232.055	−413.479	−179.633	3.128
3100	104.412	207.215	129.004	242.454	−414.153	−171.827	2.895
3193.000	105.190	210.313	131.328	252.201	CRYSTAL <--> LIQUID		
3193.000	108.784	241.762	131.328	352.617	TRANSITION		
3200	108.784	242.000	131.569	353.378	−314.303	−164.220	2.681
3300	108.784	245.348	134 967	364.257	−314.498	−159.527	2.525
3400	108.784	248.595	138.261	375.135	−314.693	−154.828	2.379
3500	108.784	251.749	141.459	386.014	−314.889	−150.124	2.240
3600	108.784	254.813	144.565	396.892	−315.084	−145.413	2.110
3700	108.784	257.794	147.586	407.770	−724.378	−132.909	1.876
3800	108.784	260.695	150.524	418.649	−723.339	−116.937	1.607
3900	108.784	263.521	153.385	429.527	−722.355	−100.993	1.353
4000	108.784	266.275	156.173	440.406	−721.426	−85.072	1.111
4100	108.784	268.961	158.892	451.284	−720.549	−69.174	0.881
4200	108.784	271.582	161.544	462.162	−1679.422	−39.249	0.488
4300	108.784	274.142	164.133	473.041	−1676.470	−0.232	0.003
4400	108.784	276.643	166.661	483.919	−1673.570	38.717	−0.460
4500	108.784	279.088	169.133	494 798	−1670.720	77.600	−0.901
4600	108.784	281.479	171.549	505.676	−1667.918	116.421	−1.322
4700	108.784	283.818	173.913	516.554	−1665.163	155.181	−1.725
4800	108.784	286.108	176.227	527.433	−1662.453	193.883	−2.110
4900	108.784	288.351	178.492	538.311	−1659 788	232.529	−2.479
5000	108.784	290.549	180.711	549.190	−1657.165	271.121	−2.832
5100	108.784	292.703	182.886	560.068	−1654.583	309.661	−3.172
5200	108.784	294.816	185.018	570.946	−1652.041	348.150	−3.497
5300	108.784	296.888	187.110	581.825	−1649.538	386.592	−3.810
5400	108.784	298.921	189.161	592.703	−1647.072	424.986	−4.111
5500	108.784	300.917	191.175	603.582	−1644.642	463.335	−4.400
5600	108.784	302.877	193.152	614.460	−1642.247	501.640	−4.679
5700	108.784	304.803	195.094	625.338	−1639.886	539.903	−4.948
5800	108.784	306.695	197.002	636.217	−1637.558	578.125	−5.207
5900	108.784	308.554	198.877	647.095	−1635.262	616.306	−5.456
6000	108.784	310.383	200.721	657.974	−1632.997	654.449	−5.697

PREVIOUS: CURRENT: June 1965

Zirconium Boride (ZrB_2) CRYSTAL $M_r = 112.84$ Zirconium Boride (ZrB_2) $B_2Zr_1(cr)$

$S°(298.15\ K) = 35.94 \pm 0.04\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 3323\ K$

$\Delta_f H°(0\ K) = -321.3 \pm 6.7\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -322.6 \pm 6.7\ kJ{\cdot}mol^{-1}$
$\Delta_{fus} H° = [104.6]\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

Johnson[1] reported $\Delta_f H°(ZrB_{1.999 \pm 0.006}$, cr, 298.15 K) = −78.7 ± 1.5 kcal mol^{-1}. Their value was obtained by fluorine bomb calorimetry and was based on their recently redetermined value of $\Delta_f H°(BF_3$, g, 298.15 K) = −271.80 ± 0.20 kcal·mol^{-1}.

Kibler *et al.*[2] studied the vaporization of $ZrB_{1.931}$ by the Knudsen effusion method. Over the range 2260 to 2500 K, log K_p = 22.038–0.164 × 10^4/T for the reaction $ZrB_{1.931}(cr) = Zr(g) + 1.931\ B(g)$. JANAF auxiliary data were used to calcuate $\Delta_r H°$(298.15 K) = 478.5 ± 1.5 kcal·mol^{-1} by the 3rd law method and $\Delta_f H°(ZrB_{1.932}$, cr, 298.15 K) = −76.7 ± 3.2 kcal·mol^{-1}.

Trulson and Goldstein[3] investigated the decomposition vapor pressure of the reaction $ZrB_2(cr) = Zr(g) + 2\ B(g)$ and reported $\Delta_f H°(ZrB_2$, cr, 298.15 K) = −72.1 ± 5.3 kcal·mol^{-1}. They also reported $\Delta_r H°$(298.15 K) = 289.7 kcal mol^{-1} for the reaction $ZrB_2(cr) + C(cr) = ZrC(cr) + 2\ B(g)$. Using the JANAF $\Delta_f H°$(ZrC, cr, 298.15 K) = −47.0 ± 3 kcal·mol^{-1}, $\Delta_f H°(ZrB_2$, cr, 298.15 K) = −76.1 ± 3 kcal·mol^{-1} was calculated. JANAF values for $\Delta_{vap} H°$(B, g, 298.15 K) and Zr(g) were not used since their independent determinations serve to cancel instrumental constants.

From oxygen bomb calorimetry, Huber *et al.*[4] reported $\Delta_f H°(ZrB_2$, cr, 298.15 K) = −77.2 ± 1.2 kcal·mol^{-1}.

$\Delta_f H°(ZrB_2$, cr, 298.15 K) = −77.1 ± 1.6 kcal·mol^{-1} was chosen as a value representative of the above.

Heat Capacity and Entropy

The heat capacity of ZrB_2(cr) has been determined by the following investigators.

	Source	Method	T/K
[5]	Adiabatic calorimetry		5–350
[6]	Copper-block drop calorimeter		410–1125
[7]	Copper-block drop calorimeter		430–1170
[8]	Arc-imaging furnace		1300–2150
[9]	Pulse-method		1740–2520
[10]	Drop type ice calorimeter		500–2500

Westrum and Feick's[5] values were adopted to 350 K. The disparities in heat capacities above room temperatures seem too great to be errors in measurement and are probably due to sample differences. Since the samples used by Westrum and Feick[5] and by Valentine *et al.*[6] were from the same batch, Valentine's data were used above 350 K. The two sets of data were fitted to a Shomate plot which was extrapolated to 4000 K. However, in consideration of the results of Mezsaki,[7] Prophet[8] and Neel *et al.*,[10] the C_p extrapolation ran somewhat higher than a direct extrapolation of Valentine's data would yield.

$S°(ZrB_2$, 298.15 K) = 8.59 cal·K^{-1}·mol^{-1} was determined by Westrum.[5]

Fusion Data

The melting point has been reported as 3313, 3323 and 3265 K by Glaser and Post,[11] Post *et al.*[12] and Greenwood,[13] respectively. The enthalpy of fusion *is derived from an estimated* $\Delta_{fus}S°$ = 2.5 *cal*·K^{-1} *g-atom*$^{-1}$ at 3323 K. It should be pointed out that an error of 0.5 cal·K^{-1} g-atom^{-1} in the estimation of $\Delta_{fus}S°$ is 5 kcal·mol^{-1} in $\Delta_{fus}H°$.

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.653	−321.314	−321.314	INFINITE
100	12.008	4.926	67.811	−6.289	−321.884	−320.909	167.626
200	32.803	19.732	39.899	−4 033	−322.488	−319.657	83.486
298.15	48.242	35.941	35.941	0.	−322.586	−318.234	55.753
300	48.488	36.240	35.941	0.089	−322.586	−318.207	55.405
400	57.505	51.582	37.972	5.444	−322.516	−316.760	41.365
500	62.634	65.010	42.068	11.471	−322.575	−315.317	32.941
600	65.810	76.725	46.889	17.902	−322.798	−313.847	27.323
700	68.028	87.043	51.903	24.598	−323.179	−312.327	23.306
800	69.710	96.240	56.881	31.487	−323.705	−310.743	20.289
900	71.090	104.534	61.723	38.530	−324.373	−309.084	17.939
1000	72.153	112.079	66.387	45.693	−325.191	−307.343	16.054
1100	73.174	119.004	70.860	52.959	−326.156	−305.512	14.508
1200	74.195	125.415	75.142	60.327	−330.967	−303.366	13.205
1300	75.216	131.394	79.242	67 798	−331.648	−301.039	12.096
1400	76.237	137.005	83.169	75.370	−332.366	−298.658	11.143
1500	77.258	142.300	86.937	83.045	−333.123	−296.224	10.315
1600	78.278	147.319	90.555	90.822	−333.926	−293.738	9.590
1700	79.299	152.095	94.036	98.701	−334.780	−291.200	8.947
1800	80.320	156.656	97.389	106.682	−335.694	−288.611	8.375
1900	81.341	161.026	100.624	114.765	−336.675	−285.969	7.862
2000	82.362	165.225	103.750	122.950	−337.731	−283.273	7.398
2100	83.383	169.268	106.774	131.237	−338.872	−280.522	6.978
2200	84.404	173.170	109.704	139.627	−361.430	−276.970	6.576
2300	85.425	176.945	112.546	148.118	−363.185	−273.091	6.202
2400	86.446	180.602	115.306	156.712	−465.422	−266.999	5.811
2500	87.467	184.152	117.989	165.407	−467.260	−258.694	5.405
2600	88.487	187.602	120.600	174.205	−468.997	−250.316	5.029
2700	89.508	190.961	123.144	183.105	−470.631	−241.874	4.679
2800	90.529	194.234	125.625	192.107	−472.163	−233.373	4.354
2900	91.550	197.429	128.046	201.211	−473.593	−224.820	4.049
3000	92.571	200.550	130.411	210.417	−474.921	−216.218	3.765
3100	93.592	203.602	132.723	219.725	−476.147	−207.575	3.498
3200	94.613	206.589	134.985	229.135	−477.271	−198.893	3.247
3300	95.634	209.516	137.199	238.647	−478.292	−190.177	3.010
3323.000	95.868	210.181	137.702	240.850	--- CRYSTAL <--> LIQUID ---		
3400	96.655	212.387	139.368	248.262	−479.212	−181.433	2.787
3500	97.675	215.203	141.495	257.978	−480.029	−172.662	2.577
3600	98.696	217.969	143.581	267.797	−480.745	−163.870	2.378
3700	99.717	220.687	145.628	277.717	−481.358	−155.059	2.189
3800	100.738	223.360	147.639	287.740	−481.869	−146.233	2.010
3900	101.759	225.990	149.614	297.865	−482.278	−137.395	1.840
4000	102.780	228.579	151.556	308.092	−482.585	−128.548	1.679

PREVIOUS: March 1963   CURRENT: June 1965

Zirconium Boride (ZrB_2) LIQUID M_r = 112.84

$S°(298.15\ K) = [64.742]\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{fus} = 3323\ K$
$T_{dcm} = [4466]\ K$

$\Delta_f H°(298.15\ K) = [-224.832]\ kJ \cdot mol^{-1}$
$\Delta_{fus} H° = [104.6]\ kJ \cdot mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(ZrB_2, l, 298.15\ K)$ is calculated from $\Delta_f H°(ZrB_2, cr, 298.15\ K)$ by adding the enthalpy of fusion, $\Delta_{fus} H°$, and the difference in enthalpy, $H°(3323\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

A glass transition is assumed at 2200 K. The heat capacities at and below 2200 K are assumed to be equal to those of ZrB_2(cr). Above 2200 K the heat capacities were estimated to be constant.

$S°(ZrB_2, l, 298.15\ K)$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Decomposition Data

T_{dcm} is estimated as the temperature for which $\Delta_r G° = 0$ for the reaction $ZrB_2(l) = Zr(g) + 2\ B(g)$.

Zirconium Boride (ZrB_2) $B_2Zr_1(l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
298.15	48.242	64.742	64.742	0.	−224.832	−229.067	40.132
300	48.488	65.041	64.743	0.089	−224.831	−229.094	39.889
400	57.505	80.383	66.774	5.444	−224.761	−230.526	30.104
500	62.634	93.812	70.869	11.471	−224.821	−231.963	24.233
600	65.810	105.527	75.691	17.902	−225.044	−233.374	20.317
700	68.028	115.845	80.705	24.598	−225.424	−234.734	17.516
800	69.710	125.042	85.683	31.487	−225.950	−236.030	15.411
900	71.090	133.335	90.524	38.530	−226.619	−237.251	13.770
1000	72.153	140.881	95.188	45.693	−227.437	−238.390	12.452
1100	73.174	147.806	99.661	52.959	−228.401	−239.440	11.370
1200	74.195	154.216	103.944	60.327	−233.213	−240.174	10.454
1300	75.216	160.196	108.043	67.798	−233.894	−240.727	9.673
1400	76.237	165.807	111.971	75.370	−234.611	−241.226	9.000
1500	77.258	171.102	115.738	83.045	−235.369	−241.672	8.416
1600	78.278	176.120	119.357	90.822	−236.171	−242.066	7.903
1700	79.299	180.896	122.837	98.701	−237.026	−242.409	7.448
1800	80.320	185.458	126.190	106.682	−237.939	−242.699	7.043
1900	81.341	189.828	129.425	114.765	−238.920	−242.937	6.679
2000	82.362	194.026	132.551	122.950	−239.977	−243.122	6.350
2100	83.383	198.069	135.575	131.237	−241.118	−243.251	6.051
2200	84.404	201.972	138.505	139.627	−263.676	−242.579	5.760
2200.000	84.404	201.972	138.505	139.627	GLASS <--> LIQUID		
2200.000	96.232	201.972	138.505	139.627	TRANSITION		
2300	96.232	206.250	141.358	149.250	−264.298	−241.606	5.487
2400	96.232	210.345	144.148	158.873	−365.506	−238.467	5.190
2500	96.232	214.274	146.875	168.496	−366 417	−233.155	4.872
2600	96.232	218.048	149.540	178.119	−367.328	−227.807	4.577
2700	96.232	221.680	152.145	187.743	−368.238	−222.423	4.303
2800	96.232	225.179	154.692	197.366	−369.149	−217.006	4.048
2900	96.232	228.556	157.181	206.989	−370 060	−211.556	3.811
3000	96.232	231.819	159.615	216.612	−370.971	−206.075	3.588
3100	96.232	234.974	161.995	226.235	−371.882	−200.564	3.379
3200	96.232	238.029	164.324	235.859	−372.792	−195.023	3.183
3300	96.232	240.991	166.602	245.482	−373.703	−189.453	2.999
3323.000	96.232	241.659	167.119	247.695	--- CRYSTAL <--> LIQUID ---		
3400	96.232	243.863	168.833	255.105	−374.614	−183.856	2.825
3500	96.232	246.653	171.016	264.728	−375.525	−178.233	2.660
3600	96.232	249.364	173.155	274.351	−376.436	−172.583	2.504
3700	96.232	252.001	175.251	283.975	−377.346	−166.908	2.356
3800	96.232	254.567	177.304	293.598	−378.257	−161.208	2.216
3900	96.232	257.067	179.318	303.221	−379.168	−155.484	2.082
4000	96.232	259.503	181.292	312.844	−380.079	−149.737	1.955
4100	96.232	261.879	183.229	322.467	−380.990	−143.967	1.834
4200	96.232	264.198	185.129	332.091	−1341.599	−124.127	1.544
4300	96.232	266.463	186.994	341.714	−1340.336	−95.155	1.156
4400	96.232	268.675	188.826	351.337	−1339.076	−66.211	0.786
4500	96.232	270.838	190.624	360.960	−1337.820	−37.297	0.433
4600	96.232	272.953	192.391	370.583	−1336.568	−8.410	0.095
4700	96.232	275.022	194.127	380.207	−1335.322	20.449	−0.227
4800	96.232	277.048	195.834	389.830	−1895.018	60.900	−0.663
4900	96.232	279.032	197.511	399.453	−1893.436	101.632	−1.083
5000	96.232	280.977	199.161	409.076	−1891.877	142.331	−1.487

PREVIOUS: December 1962 CURRENT: June 1965

Zirconium Boride (ZrB_2) CRYSTAL-LIQUID

0 to 3323 K		crystal
above	3323 K	liquid

Refer to the individual tables for details.

$M_r = 112.84$ Zirconium Boride (ZrB_2) $B_2Zr_1(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.653	−321.314	−321.314	INFINITE
100	12.008	4.926	67.811	−6.289	−321.884	−320.909	167.626
200	32.803	19.732	39.899	−4.033	−322.488	−319.657	83.486
298.15	48.242	35.941	35.941	0.	−322.586	−318.234	55.753
300	48.488	36.240	35.941	0.089	−322.586	−318.207	55.405
400	57.505	51.582	37.972	5.444	−322.516	−316.760	41.365
500	62.634	65.010	42.068	11.471	−322.575	−315.317	32.941
600	65.810	76.725	46.889	17.902	−322.798	−313.847	27.323
700	68.028	87.043	51.903	24.598	−323.179	−312.327	23.306
800	69.710	96.240	56.881	31.487	−323.705	−310.743	20.289
900	71.090	104.534	61.723	38.530	−324.373	−309.084	17.939
1000	72.153	112.079	66.387	45.693	−325.191	−307.343	16.054
1100	73.174	119.004	70.860	52.959	−326.156	−305.512	14.508
1200	74.195	125.415	75.142	60.327	−330.967	−303.366	13.205
1300	75.216	131.394	79.242	67.798	−331.648	−301.039	12.096
1400	76.237	137.005	83.169	75.370	−332.366	−298.658	11.143
1500	77.258	142.300	86.937	83.045	−333.123	−296.224	10.315
1600	78.278	147.319	90.555	90.822	−333.926	−293.738	9.590
1700	79.299	152.095	94.036	98.701	−334.780	−291.200	8.947
1800	80.320	156.656	97.389	106.682	−335.694	−288.611	8.375
1900	81.341	161.026	100.624	114.765	−336.675	−285.969	7.862
2000	82.362	165.225	103.750	122.950	−337.731	−283.273	7.398
2100	83.383	169.268	106.774	131.237	−338.872	−280.522	6.978
2200	84.404	173.170	109.704	139.627	−361.430	−276.970	6.576
2300	85.425	176.945	112.546	148.118	−363.185	−273.091	6.202
2400	86.446	180.602	115.306	156.712	−465.422	−266.999	5.811
2500	87.467	184.152	117.989	165.407	−467.260	−258.694	5.405
2600	88.487	187.602	120.600	174.205	−468.997	−250.316	5.029
2700	89.508	190.961	123.144	183.105	−470.631	−241.874	4.679
2800	90.529	194.234	125.625	192.107	−472.163	−233.373	4.354
2900	91.550	197.429	128.046	201.211	−473.593	−224.820	4.049
3000	92.571	200.550	130.411	210.417	−474.921	−216.218	3.765
3100	93.592	203.602	132.723	219.725	−476.147	−207.575	3.498
3200	94.613	206.589	134.985	229.135	−477.271	−198.893	3.247
3300	95.634	209.516	137.199	238.647	−478.292	−190.177	3.010
3323.000	95.868	210.181	137.702	240.850	CRYSTAL <--> LIQUID TRANSITION		
3323.000	96.232	241.659	137.702	345.450			
3400	96.232	243.863	140.081	352.859	−374.614	−183.856	2.825
3500	96.232	246.653	143.087	362.483	−375.525	−178.233	2.660
3600	96.232	249.364	146.001	372.106	−376.436	−172.583	2.504
3700	96.232	252.001	148.831	381.729	−377.346	−166.908	2.356
3800	96.232	254.567	151.580	391.352	−378.257	−161.208	2.216
3900	96.232	257.067	154.252	400.975	−379.168	−155.484	2.082
4000	96.232	259.503	156.853	410.599	−380.079	−149.737	1.955
4100	96.232	261.879	159.386	420.222	−380.990	−143.967	1.834
4200	96.232	264.198	161.854	429.845	−1341.599	−124.127	1.544
4300	96.232	266.463	164.261	439.468	−1340.336	−95.154	1.156
4400	96.232	268.675	166.609	449.091	−1339.076	−66.211	0.786
4500	96.232	270.837	168.901	458.715	−1337.820	−37.297	0.433
4600	96.232	272.953	171.140	468.338	−1336.568	−8.410	0.095
4700	96.232	275.022	173.328	477.961	−1335.322	20.449	−0.227
4800	96.232	277.048	175.468	487.584	−1895.018	60.900	−0.663
4900	96.232	279.032	177.561	497.207	−1893.436	101.632	−1.083
5000	96.232	280.977	179.610	506.831	−1891.877	142.331	−1.487

PREVIOUS: CURRENT: June 1965

Trichloroboroxin ((BOCl)$_3$) IDEAL GAS M_r = 186.7872 Trichloroboroxin (B$_3$O$_3$Cl$_3$) B$_3$Cl$_3$O$_3$(g)

$S°(298.15 \text{ K}) = [382.38] \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = -1627 \pm 8 \text{ kJ·mol}^{-1}$

$\Delta_f H°(298.15 \text{ K}) = -1632 \pm 8 \text{ kJ·mol}^{-1}$

Vibrational Frequencies and Degeneracies		
υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}
[807] (1)	[980] (2)	[600] (1)
[690] (1)	[1300] (2)	[140] (1)
[333] (1)	[920] (2)	[400] (2)
[1037] (1)	[390] (2)	[120] (2)
[400] (1)	[150] (2)	

Ground State Quantum Weight: [1] $\sigma = 6$
Point Group: [D$_{3h}$]
Bond Distances: B–Cl = [1.75] Å; B–O = [1.36] Å
Bond Angles: Cl–B–O = [120]°; B–O–B = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = [1.868800 \times 10^{-111}] \text{ g}^3\text{·cm}^6$

Enthalpy of Formation

The equilibrium constants for the reaction $B_2O_3(l) + BCl_3(g) = (BOCl)_3(g)$ were determined by Blauer and Farber in the temperature range 536–825 K by a transpiration method,[1] and in the temperature range 1234–1309 K by an effusion method.[2] Using the reported equilibrium constants, the enthalpy changes for this reaction were evaluated by both the 2nd and 3rd law methods.

Method Used	$\Delta_r H°(298.15 \text{ K})$, kcal·mol^{-1} 3rd law	2nd law	$\Delta_f H°(293.15 \text{ K})$ kcal·mol^{-1}
Transpiration	5.31	5.07 ± 0.4	−390 ± 2
Effusion	12.57	5.85 ± 3.3	−386 ± 3

By a mass spectroscopic method the enthalpy change $\Delta_r H°(1000 \text{ F}) = 16.6 \pm 2.5 \text{ kcal mol}^{-1}$, for the reaction $BCl_3(g) + B_2O_3(l) = (BOCl)_3(g)$ was determined by Porter and Gupta.[3] The $\Delta_f H°(298.15 \text{ K})$ value for (BOCl)$_3$(g) was derived as $-377 \pm 3 \text{ kcal·mol}^{-1}$. However, it is possible that the intensity of $B_3O_3Cl_3^+$, employed to plot the ion ratios $I(B_3O_3Cl_3^+)/I(BCl_2^+)$ versus $1/T$, does not fully reflect the concentration of B$_3$O$_3$Cl$_3$ especially at the highest temperatures, due to changes in the fragmentation pattern with temperature.

The value of $\Delta_f H°(298.15 \text{ K})$ adopted for (BOCl)$_3$(g) is $390 \pm 2 \text{ kcal·mol}^{-1}$ derived from transpiration data. The effusion data were measured in the temperature range where Porter and Gupta[3] found the presence of (BOCl)$_4$(g). However, this point was not taken into consideration in the report. Hence, the corresponding $\Delta_f H°(298.15 \text{ K})$ value was not adopted.

Heat Capacity and Entropy

The vibration frequencies are estimated by comparison with related molecules such as $B_3O_3F_3(g)$ and $(BH_2O)_3(g)$. The B–Cl bond distance is assumed to be the same as that in BCl$_3$(g). The B–O bond distance and all bond angles are estimated. The principal moments of inertia are: $I_A = I_B = 97.7637 \times 10^{-39}$, and $I_C = 195.5274 \times 10^{-39} \text{ g·cm}^2$.

References

[1] J. Blauer and M. Farber, J. Chem. Phys. 39, 158 (1963).
[2] J. Blauer and M. Farber, Trans. Faraday Soc. 60, 301 (1964).
[3] R. F. Porter and S. K. Gupta, J. Phys. Chem. 68, 280 (1964).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K$_f$
0	0.	0.	INFINITE	−25.342	−1626.664	−1626.664	INFINITE
100	70.079	275.129	480.665	−20.554	−1630.672	−1603.746	837.711
200	105.432	335.190	393.615	−11.685	−1631.726	−1576.278	411.682
250	119.582	360.271	384.479	−6.052	−1631.820	−1562.401	326.446
298.15	131.525	382.378	382.378	0.	−1631.760	−1549.034	271.384
300	131.953	383.193	382.381	0.244	−1631.755	−1548.521	269.622
350	142.628	404.357	384.028	7.115	−1631.558	−1534.663	229.036
400	151.707	424.012	387.812	14 480	−1631.268	−1520.839	198.601
450	159.351	442.335	392.864	22.262	−1630.909	−1507.057	174.935
500	165.756	459.466	398.677	30.394	−1630.492	−1493.317	156.006
600	175.618	490.611	411.458	47.492	−1629.526	−1465.970	127.624
700	182.610	518.238	424.777	65.423	−1628.450	−1438.795	107.364
800	187.665	542.970	438.032	83.950	−1627.326	−1411.778	92.180
900	191.400	565.300	450.953	102.912	−1626.198	−1384.903	80.378
1000	194.220	585.618	463.419	122.199	−1625.095	−1358.152	70.943
1100	196.392	604.236	475.386	141.735	−1624.038	−1331.509	63.228
1200	198.095	621.400	486.848	161.462	−1623.043	−1304.960	56.803
1300	199.452	637.311	497.818	181.342	−1622.121	−1278.491	51.370
1400	200.549	652.134	508.317	201.344	−1621.281	−1252.090	46.716
1500	201.448	666.002	518.372	221.445	−1620.531	−1225.746	42.684
1600	202.193	679.028	528.010	241.628	−1619.878	−1199.449	39.158
1700	202.817	691.305	537.258	261.880	−1619.325	−1173.189	36.048
1800	203.344	702.913	546.141	282.188	−1618.881	−1146.960	33.284
1900	203.793	713.919	554.685	302.546	−1618.548	−1120.751	30.812
2000	204.179	724.383	562.910	322.945	−1618.331	−1094.558	28.587
2100	204.513	734.353	570.839	343.380	−1618.235	−1068.372	26.574
2200	204.804	743.874	578.489	363.846	−1618.263	−1042.187	24.745
2300	205.059	752.983	585.879	384.340	−1618.419	−1015.999	23.074
2400	205.283	761.715	593.025	404.857	−1769.485	−986.595	21.473
2500	205.482	770.100	599.941	425.395	−1770.141	−953.961	19.932
2600	205.658	778.162	606.642	445.953	−1770.836	−921.301	18.509
2700	205.816	785.927	613.139	466.526	−1771.573	−888.612	17.191
2800	205.957	793.415	619.445	487.115	−1772.354	−855.895	15.967
2900	206.085	800.644	625.569	507.717	−1773.181	−823.151	14.827
3000	206.200	807.633	631.522	528.332	−1774.054	−790.376	13.762
3100	206.304	814.396	637.313	548.957	−1774.973	−757.571	12.765
3200	206.399	820.947	642.949	569.592	−1775.937	−724.738	11.830
3300	206.485	827.300	648.440	590.236	−1776.945	−691.872	10.951
3400	206.564	833.465	653.792	610.889	−1777.995	−658.975	10.124
3500	206.636	839.454	659.011	631.549	−1779.084	−626.048	9.343
3600	206.703	845.276	664.105	652.216	−1780.209	−593.087	8.605
3700	206.764	850.940	669.078	672.889	−1781.367	−560.097	7.907
3800	206.821	856.455	673.937	693.569	−1782.554	−527.072	7.245
3900	206.873	861.828	678.686	714.253	−1783.765	−494.017	6.617
4000	206.921	867.066	683.330	734.943	−1784.998	−460.932	6.019
4100	206.966	872.176	687.874	755.638	−1786.247	−427.814	5.450
4200	207.008	877.164	692.322	776.336	−3227.058	−373.594	4.646
4300	207.047	882.035	696.678	797.039	−3225.067	−305.678	3.713
4400	207.083	886.796	700.945	817.746	−3223.088	−237.809	2.823
4500	207.117	891.450	705.126	838.456	−3221.115	−169.984	1.973
4600	207.149	896.003	709.227	859.169	−3219.148	−102.203	1.161
4700	207.179	900.458	713.248	879.885	−3217.183	−34.465	0.383
4800	207.207	904.820	717.194	900.605	−3215.219	33.232	−0.362
4900	207.233	909.093	721.067	921.327	−3213.255	100.889	−1.075
5000	207.258	913.280	724.869	942.051	−3211.289	168.504	−1.760
5100	207.281	917.384	728.604	962.778	−3209.321	236.082	−2.418
5200	207.303	921.409	732.273	983.508	−3207.349	303.617	−3.050
5300	207.324	925.358	735.879	1004.239	−3205.375	371.118	−3.658
5400	207.343	929.234	739.424	1024.972	−3203.398	438.580	−4.242
5500	207.362	933.039	742.910	1045.708	−3201.419	506.006	−4.806
5600	207.380	936.775	746.338	1066.445	−3199.440	573.397	−5.348
5700	207.396	940.446	749.712	1087.183	−3197.462	640.750	−5.872
5800	207.412	944.053	753.031	1107.924	−3195.485	708.072	−6.377
5900	207.427	947.599	756.299	1128.666	−3193.512	775.355	−6.864
6000	207.441	951.085	759.517	1149.409	−3191.547	842.608	−7.336

PREVIOUS· March 1965 (1 atm) CURRENT: March 1965 (1 bar)

Trichloroboroxin (B$_3$O$_3$Cl$_3$) B$_3$Cl$_3$O$_3$(g)

Fluoroboroxin ($B_3O_3H_2F$) IDEAL GAS M_r = 101.442483 Fluoroboroxin ($B_3H_2O_3F$) $B_3F_1H_2O_3(g)$

$S°(298.15\ K) = [314.84]\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = -1587 \pm 25\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -1598 \pm 25\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
[2100] (1)	[880] (1)	[350] (1)
[870] (1)	[1460] (1)	[225] (1)
[670] (1)	[520] (1)	[800] (1)
[2200] (1)	[2230] (1)	[225] (1)
[1390] (1)	[1390] (1)	[840] (1)
[1200] (1)	[1200] (1)	[800] (1)
[880] (1)	[350] (1)	[260] (1)

Ground State Quantum Weight: [1] $\sigma = 2$
Point Group: [C_{2v}]
Bond Distances: B–O = [1.36] Å; B–H = [1.18] Å; B–F = [1.41] Å
Bond Angles: B–O–B = [120]°; O–B–H = [120]°; O–B–F = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = [2.164977 \times 10^{-113}]\ g^3 \cdot cm^6$

Enthalpy of Formation

The equilibrium constants (K), 1246–1326 K, for the two reactions $2B_3O_3F_2H(g) = B_3O_3FH_2(g) + B_3O_3F_3(g)$ and $2B_3O_3FH_2(g) = B_3O_3H_3(g) + B_3O_3F_2H(g)$ were reported by Porter and Sholette.[1] The $\Delta_f H°(298.15\ K)$ for $B_3O_3H_2F(g)$ adopted was evaluated by use of K values slightly outside the ranges given by Porter and Sholette. See the table for $B_3O_3F_2H(g)$ for details.

Heat Capacity and Entropy

The structure is assumed to be a planar six membered ring structure of C_{2v} symmetry, which has 21 vibrations of the type $8A_1$, $7B_1$, $2A_2$, and $4B_2$. These frequencies are estimated from the values for boroxin and trifluoroboroxin, the symmetry being reduced from D_{3h} as follows: $3A'_1 \rightarrow 3A_1$, $2A'_2 \rightarrow 2B_1$, $5E' \rightarrow 5A_1 + 5B_1$, $2A_2 \rightarrow 2B_2$ and $2E'' \rightarrow 2A_2 + 2B_2$.

The B–F distance is taken as approximately equal to that in $(CH_3)_2O\ BF_3$ reported by Bauer, Findlay and Laubengayer.[2] The other bond lengths and angles are taken equal to those in boroxin. The principal moments of inertia are: $I_A = 13.9711 \times 10^{-39}$, $I_B = 32.9946 \times 10^{-39}$, and $I_C = 46.9657 \times 10^{-39}\ g \cdot cm^2$.

References

[1] R. F. Porter and W. P. Sholette, J. Chem. Phys. 37, 198 (1962).
[2] S. H. Bauer, G. R. Findlay, and A. W. Laubengayer, J. Am. Chem. Soc. 67, 339 (1945).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−17.877	−1586.619	−1586.619	INFINITE
100	46.702	241.315	383.279	−14.196	−1591.820	−1571.271	820.748
200	72.105	281.675	322.817	−8.228	−1595.375	−1549.266	404.627
250	84.135	299.063	316.347	−4.321	−1596.915	−1537.558	321.255
298.15	95.245	314.841	314.841	0.	−1598.288	−1526.000	267.349
300	95.659	315.432	314.843	0.177	−1598.338	−1525.551	265.622
350	106.362	330.993	316.047	5.231	−1599.624	−1513.316	225.850
400	116.099	345.842	318.851	10.797	−1600.778	−1500.906	195.998
450	124.856	360.032	322.644	16.825	−1601.803	−1488.359	172.764
500	132.685	373.600	327.066	23.267	−1602.695	−1475.705	154.166
600	145.879	399.004	336.970	37.220	−1604.090	−1450.168	126.248
700	156.339	422.308	347.520	52.351	−1605.020	−1424.435	106.293
800	164.653	443.748	358.227	68.417	−1605.565	−1398.596	91.319
900	171.295	463.539	368.843	85.226	−1605.811	−1372.708	79.670
1000	176.637	481.873	379.241	102.633	−1605.833	−1346.804	70.350
1100	180.969	498.919	389.355	120.520	−1605.698	−1320.907	62.725
1200	184.511	514.822	399.155	138.800	−1605.459	−1295.026	56.371
1300	187.433	529.710	408.631	157.402	−1605.162	−1269.169	50.996
1400	189.864	543.692	417.784	176.270	−1604.842	−1243.335	46.389
1500	191.902	556.862	426.621	195.362	−1604.529	−1217.525	42.398
1600	193.625	569.304	435.154	214.640	−1604.246	−1191.734	38.906
1700	195.093	581.088	443.395	234.078	−1604.010	−1165.959	35.826
1800	196.351	592.275	451.358	253.652	−1603.838	−1140.197	33.088
1900	197.436	602.921	459.057	273.343	−1603.740	−1114.442	30.638
2000	198.379	613.073	466.506	293.134	−1603.725	−1088.690	28.434
2100	199.202	622.772	473.718	313.014	−1603.800	−1062.937	26.439
2200	199.924	632.056	480.706	332.971	−1603.970	−1037.177	24.626
2300	200.562	640.958	487.481	352.996	−1604.238	−1011.409	22.970
2400	201.126	649.506	494.055	373.081	−1755.386	−982.420	21.382
2500	201.629	657.726	500.439	393.220	−1756.092	−950.199	19.853
2600	202.078	665.643	506.641	413.405	−1756.805	−917.949	18.442
2700	202.481	673.277	512.672	433.634	−1757.525	−885.671	17.134
2800	202.844	680.648	518.541	453.900	−1758.253	−853.367	15.920
2900	203.172	687.772	524.254	474.201	−1758.990	−821.037	14.788
3000	203.469	694.665	529.820	494.534	−1759.736	−788.681	13.732
3100	203.739	701.341	535.246	514.894	−1760.491	−756.300	12.744
3200	203.985	707.813	540.538	535.280	−1761.256	−723.895	11.816
3300	204.209	714.094	545.703	555.690	−1762.029	−691.466	10.945
3400	204.415	720.193	550.745	576.122	−1762.810	−659.012	10.124
3500	204.605	726.121	555.672	596.573	−1763.601	−626.537	9.351
3600	204.779	731.888	560.487	617.042	−1764.399	−594.038	8.619
3700	204.939	737.501	565.196	637.528	−1765.206	−561.517	7.927
3800	205.088	742.968	569.802	658.030	−1766.022	−528.973	7.271
3900	205.225	748.297	574.311	678.545	−1766.846	−496.408	6.649
4000	205.353	753.495	578.726	699.074	−1767.679	−463.823	6.057
4100	205.471	758.567	583.051	719.616	−1768.521	−431.216	5.494
4200	205.582	763.519	587.289	740.168	−3208.919	−377.516	4.695
4300	205.685	768.358	591.444	760.732	−3206.518	−310.129	3.767
4400	205.781	773.088	595.518	781.305	−3204.132	−242.800	2.882
4500	205.871	777.713	599.516	801.888	−3201.763	−175.524	2.037
4600	205.955	782.239	603.439	822.479	−3199.411	−108.301	1.230
4700	206.034	786.669	607.291	843.079	−3197.080	−41.127	0.457
4800	206.109	791.008	611.073	863.686	−3194.769	25.996	−0.283
4900	206.178	795.258	614.789	884.300	−3192.481	93.073	−0.992
5000	206.244	799.424	618.440	904.921	−3190.217	160.102	−1.673
5100	206.306	803.509	622.029	925.549	−3187.980	227.086	−2.326
5200	206.365	807.516	625.558	946.182	−3185.771	294.025	−2.954
5300	206.420	811.447	629.028	966.822	−3183.591	360.925	−3.557
5400	206.472	815.306	632.442	987.466	−3181.445	427.782	−4.138
5500	206.522	819.095	635.801	1008.116	−3179.332	494.599	−4.697
5600	206.569	822.817	639.108	1028.771	−3177.256	561.380	−5.236
5700	206.613	826.473	642.363	1049.430	−3175.219	628.123	−5.756
5800	206.655	830.067	645.568	1070.093	−3173.222	694.832	−6.258
5900	206.696	833.600	648.725	1090.761	−3171.268	761.503	−6.742
6000	206.734	837.074	651.836	1111.432	−3169.360	828.145	−7.210

PREVIOUS December 1965 (1 atm) CURRENT. December 1965 (1 bar)

Difluoroboroxin ($B_3O_3HF_2$) IDEAL GAS $M_r = 119.432946$ Difluoroboroxin ($B_3HO_3F_2$) $B_3F_2H_1O_3(g)$

$S°(298.15 K) = [328.99] J·K^{-1}·mol^{-1}$

$\Delta_f H°(0 K) = -1977 \pm 21 kJ·mol^{-1}$
$\Delta_f H°(298.15 K) = -1987 \pm 21 kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm $^{-1}$	ν, cm $^{-1}$	ν, cm $^{-1}$
[1650] (1)	[660] (1)	[300] (1)
[830] (1)	[1370] (1)	[220] (1)
[610] (1)	[490] (1)	[710] (1)
[1800] (1)	[1840] (1)	[220] (1)
[1385] (1)	[1385] (1)	[780] (1)
[1080] (1)	[1080] (1)	[700] (1)
[660] (1)	[310] (1)	[230] (1)

Ground State Quantum Weight: [1] $\sigma = 2$
Point Group: $[C_{2v}]$
Bond Distances: B–O = [1.36] Å; B–H = [1.18] Å; B–F = [1.41] Å
Bond Angles: B–O–B = [120]°, O–B–H = [120]°; O–B–F = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = [7.586853 \times 10^{-113}] g^3·cm^6$

Enthalpy of Formation

The stabilities of gaseous boroxin ($B_3O_3H_3$) and its fluoro derivatives have been studied by Porter and Sholette.[1] From the mass spectra of the gaseous reaction products generated by reaction of an H_2–BF_3 mixture on B_2O_3 at 1250 K, the equilibrium constants (K) for the following proposed reactions were reported.

Reaction	T/K	K	$\Delta_r H°(298.15 K)$, kcal·mol^{-1}
(1) $H_2(g) + B_3O_3F_3(g) = HF(g) + B_3O_3F_2H(g)$	1246–1326	4.2×10^{-3}–2.3×10^{-2}	20.45–17.17
(2) $2B_3O_3F_2H(g) = B_3O_3FH_2(g) + B_3O_3F_3(g)$	1246–1326	0.62–0.46	1.28–2.15
(3) $2B_3O_3FH_2(g) = B_3O_3H_3(g) + B_3O_3F_2H(g)$	1246–1326	1.0–0.63	−2.56–−1.51

Using these reported K values the corresponding enthalpy changes are evaluated by the 3rd law method. The results obtained are listed in the above table. Based on $\Delta_f H°(298.15 K) = -565.3$ and -64.8 kcal·mol^{-1} for $B_3O_3F_3(g)$ and HF(g), respectively, the value of $\Delta_f H°(298.15 K)$ for $B_3O_3F_2H(g)$ is calculated from Reaction (1) as -482 kcal·mol^{-1}. From Reaction (2), the $\Delta_f H°(298.15 K)$ value for $B_3O_3FH_2(g)$ is calculated as -397 kcal·mol^{-1}. However, employing $\Delta_f H°(B_3O_3H_3, g, 298.15 K) = -291$ kcal·mol^{-1}, the values of $\Delta_f H°(298.15 K)$ for $B_3O_3FH_2(g)$ and $B_3O_3F_2H(g)$ thus obtained do not fit properly for Reaction (3). Therefore, the $\Delta_f H°(298.15 K)$ for $B_3O_3FH_2(g)$ and $B_3O_3F_2H(g)$ adopted are evaluated by use of K values slightly outside the ranges given by Porter and Sholette.[1]

Heat Capacity and Entropy

The vibrational frequencies are obtained by comparison with $B_3O_3F_3(g)$ and $B_3H_3O_3(g)$. The types of vibration and symmetry are identical to those given for $B_3O_3H_2F(g)$. The bond angles and lengths are taken equal to those for $B_3O_3H_2F(g)$. The principal moments of inertia are: $I_A = 22.0494 \times 10^{-39}$, $I_B = 48.6611 \times 10^{-39}$, and $I_C = 70.7105 \times 10^{-39}$ g·cm^2.

Reference

[1] R. F. Porter and W. P. Sholette, J. Chem. Phys. 37, 198 (1962).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−19.127	−1976.801	−1976.801	INFINITE
100	49.248	249.646	403.289	−15.364	−1981.875	−1958.677	1023.108
200	78.340	292.875	337.680	−8.961	−1985.112	−1934.119	505.140
250	91.721	311.813	330.633	−4.705	−1986.357	−1921.223	401.418
298.15	103.528	328.994	328.994	0.	−1987.400	−1908.582	334.376
300	103.959	329.636	328.996	0.192	−1987.437	−1908.093	332.228
350	114.983	346.504	330.303	5.670	−1988.368	−1894.793	282.782
400	124.838	362.514	333.337	11.671	−1989.175	−1881.368	245.682
450	133.599	377.734	337.432	18.136	−1989.866	−1867.850	216.814
500	141.353	392.220	342.192	25.014	−1990.440	−1854.261	193.713
600	154.206	419.177	352.812	39.819	−1991.256	−1826.941	159.049
700	164.136	443.727	364.073	55.758	−1991.685	−1799.516	134.282
800	171.816	466.168	375.453	72.572	−1991.811	−1772.052	115.703
900	177.795	486.764	386.693	90.064	−1991.713	−1744.586	101.253
1000	182.495	505.750	397.662	108.088	−1991.461	−1717.140	89.694
1100	186.231	523.325	408.297	126.531	−1991.110	−1689.724	80.238
1200	189.236	539.663	418.571	145.310	−1990.706	−1662.343	72.360
1300	191.679	554.909	428.479	164.360	−1990.286	−1634.997	65.695
1400	193.686	569.190	438.025	183.631	−1989.876	−1607.682	59.983
1500	195.353	582.612	447.221	203.086	−1989.501	−1580.396	55.034
1600	196.750	595.265	456.082	222.693	−1989.178	−1553.133	50.705
1700	197.930	607.230	464.625	242.428	−1988.921	−1525.889	46.885
1800	198.936	618.572	472.865	262.273	−1988.740	−1498.658	43.490
1900	199.799	629.352	480.820	282.211	−1988.645	−1471.434	40.453
2000	200.544	639.620	488.505	302.229	−1988.639	−1444.212	37.719
2100	201.193	649.420	495.936	322.317	−1988.727	−1416.990	35.246
2200	201.760	658.793	503.127	342.465	−1988.911	−1389.759	32.997
2300	202.258	667.773	510.092	362.666	−1989.192	−1362.520	30.944
2400	202.699	676.391	516.843	382.915	−2140.347	−1332.059	28.992
2500	203.090	684.673	523.391	403.204	−2141.054	−1298.366	27.128
2600	203.439	692.645	529.749	423.531	−2141.758	−1264.645	25.407
2700	203.751	700.329	535.925	443.891	−2142.458	−1230.896	23.813
2800	204.032	707.744	541.930	464.280	−2143.152	−1197.121	22.333
2900	204.285	714.909	547.772	484.696	−2143.840	−1163.323	20.954
3000	204.513	721.838	553.459	505.136	−2144.520	−1129.500	19.666
3100	204.721	728.548	559.000	525.598	−2145.191	−1095.654	18.462
3200	204.910	735.050	564.400	546.080	−2145.852	−1061.789	17.332
3300	205.083	741.358	569.667	566.580	−2146.502	−1027.902	16.270
3400	205.241	747.483	574.808	587.096	−2147.138	−993.995	15.271
3500	205.386	753.435	579.827	607.628	−2147.762	−960.070	14.328
3600	205.519	759.222	584.730	628.173	−2148.371	−926.127	13.438
3700	205.642	764.855	589.522	648.731	−2148.966	−892.168	12.595
3800	205.756	770.341	594.209	669.301	−2149.547	−858.192	11.797
3900	205.861	775.687	598.794	689.882	−2150.112	−824.201	11.039
4000	205.958	780.900	603.282	710.473	−2150.663	−790.197	10.319
4100	206.049	785.987	607.676	731.073	−2151.199	−756.179	9.634
4200	206.133	790.953	611.981	751.683	−3591.269	−701.075	8.719
4300	206.211	795.804	616.200	772.300	−3588.516	−632.293	7.681
4400	206.285	800.546	620.336	792.925	−3585.755	−563.576	6.691
4500	206.353	805.182	624.392	813.557	−3582.988	−494.922	5.745
4600	206.417	809.719	628.372	834.195	−3580.217	−426.329	4.841
4700	206.477	814.158	632.278	854.840	−3577.444	−357.796	3.976
4800	206.534	818.506	636.112	875.490	−3574.670	−289.322	3.148
4900	206.587	822.765	639.878	896.147	−3571.898	−220.905	2.355
5000	206.637	826.939	643.578	916.808	−3569.129	−152.545	1.594
5100	206.684	831.032	647.213	937.474	−3566.367	−84.241	0.863
5200	206.729	835.046	650.787	958.145	−3563.614	−15.992	0.161
5300	206.771	838.984	654.301	978.819	−3560.872	52.207	−0.515
5400	206.810	842.849	657.757	999.499	−3558.145	120.352	−1.164
5500	206.848	846.644	661.157	1020.181	−3555.435	188.446	−1.790
5600	206.883	850.372	664.502	1040.868	−3552.744	256.494	−2.392
5700	206.917	854.034	667.796	1061.558	−3550.076	324.491	−2.974
5800	206.949	857.633	671.038	1082.251	−3547.434	392.444	−3.534
5900	206.980	861.171	674.230	1102.948	−3544.820	460.348	−4.076
6000	207.009	864.650	677.375	1123.647	−3542.238	528.212	−4.598

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

Trifluoroboroxin ((BOF)$_3$) CRYSTAL M_r = 137.423409 Trifluoroboroxin ($B_3O_3F_3$) $B_3F_3O_3$(cr)

$S°$(298.15 K) = [217.6] J·K^{-1}·mol^{-1}
T_{fus} = 353 K

$\Delta_f H°$(0 K) = Unknown
$\Delta_f H°$(298.15 K) = −2454 ± 12 kJ·mol^{-1}
$\Delta_{fus}H°$ = Unknown

Enthalpy of Formation

The enthalpies of solution of the compounds: B_2O_3(gl), BF_3(g) and (BOF)$_3$(cr) in water and methanol, respectively, were reported by Magee.[1] The corresponding enthalpy changes for the reaction B_2O_3(gl) + BF_3(g) = (BOF)$_3$(cr) were derived as −19.8 and −14.4 kcal·mol^{-1}, yielding $\Delta_f H°$(298.15 K) values for (BOF)$_3$(cr) as −589.18 and −583.78 kcal·mol^{-1}, respectively. The adopted value of $\Delta_f H°$(298.15 K) for (BOF)$_3$(cr) is the average of these two values obtained.

Heat Capacity and Entropy

The heat capacities for (BOF)$_3$(cr) are estimated from the C_p values for B_2O_3(cr) and BF_3(g), according to the method suggested by Kubaschewski and Evans.[2]

$S°$(298.15 K) for (BOF)$_3$(cr) was estimated by Magee.[1]

Fusion Data

The value of T_{fus} was reported by Magee.[1]

Sublimation Data

The enthalpy of sublimation for (BOF)$_3$(cr) is calculated as the difference in $\Delta_f H°$(298.15 K) between the crystal and gas.

References

[1] E. M. Magee, J. Inorg. Nucl. Chem. 22, 156 (1961).
[2] O. Kubaschewski and E. Ll. Evans, "Metallurgical Thermochemistry," 3rd ed., Pergamon Press, New York, 426 pp. (1958).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	125.520	217.568	217.568	0.	−2453.916	−2331.126	408.404
300	125.874	218.346	217.570	0.233	−2453.915	−2330.364	405.753
400	144.766	257.156	222.735	13.769	−2453.752	−2289.199	298.939
500	163.176	291.484	233.111	29.187	−2453.164	−2248.116	234.859
600	178.761	322.641	245.476	46.299	−2451.944	−2207.210	192.155
700	192.464	351.250	258.570	64.876	−2450.042	−2166.562	161.671
800	204.284	377.743	271.831	84.729	−2447.457	−2126.234	138.829
900	214.221	402.396	284.985	105.670	−2444.251	−2086.267	121.084
1000	222.170	425.393	297.889	127.504	−2440.532	−2046.687	106.908
1100	228.446	446.875	310.468	150.048	−2436.420	−2007.498	95.328
1200	232.840	466.950	322.681	173.123	−2432.054	−1968.696	85.695
1300	235.978	485.720	334.508	196.575	−2427.556	−1930.265	77.559
1400	237.860	503.284	345.943	220.277	−2423.029	−1892.182	70.598
1500	238.488	519.723	356.987	244.105	−2418.582	−1854.421	64.577

PREVIOUS: September 1962   CURRENT: March 1965

Trifluoroboroxin ((BOF)$_3$) **IDEAL GAS** **M_r = 137.423409** **Trifluoroboroxin (B$_3$O$_3$F$_3$)** **B$_3$F$_3$O$_3$(g)**

$S°(298.15\ K) = [342.45]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -2357.0 \pm 4.2\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -2365.2 \pm 4.2\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

ν, cm^{-1}	ν, cm^{-1}	ν, cm^{-1}
[1233] (1)	1450 (2)	714 (1)
[790] (1)	1381 (2)	[170] (1)
[570] (1)	966 (2)	[630] (2)
[1280] (1)	[420] (2)	[185] (2)
[440] (1)	[220] (2)	

Ground State Quantum Weight: [1] $\sigma = 6$
Point Group: [D$_{3h}$]
Bond Distances: B–F = [1.3] Å; B–O = [1.36] Å
Bond Angles: F–B–O = [120]°; B–O–B = [120]°, O–B–O = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = [1.925790 \times 10^{-113}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpy changes of the reaction $B_2O_3(l) + BF_3(g) = (BOF)_3(g)$ are derived by both the 2nd and 3rd law methods, using the equilibrium constant data reported by several investigators.

Source	$\Delta_r H°$(298.15 K), kcal·mol^{-1} 3rd law	2nd law	$\Delta_f H°$(298.15 K) kcal mol^{-1}
Hildenbrand, *et al.*[1]	4.06	4.01 ± 0.3	−565.32 ± 1.0
Fisher, *et al.*[2]	3.41	6.45 ± 0.6	−565.97 ± 1.5
Smith and Lawrence[3]	4.03	—	−565.35 ± 1.3
Farber[4]	5.25	—	−565.13 ± 2.0
	2.56	7.58 ± 0.2	−565.82 ± 2.0
Porter, *et al.*[5]	—	4.33 ± 0.30	−565.05 ± 1.0

The adopted value of $\Delta_f H°$(298.15 K) for (BOF)$_3$(cr) is the weighted average of the six $\Delta_f H°$(298.15 K) values listed above.

Heat Capacity and Entropy

The infra-red spectrum has been reported by Smith and Lawrence[3] and by Fisher, Lehmann, and Shapiro[6] who also made a partial assignment. The unassigned bands at 1280 and 1233 from Fisher, *et al.*,[6] can be assigned to the A_2' and A_1' species which may be observed if the selection rules are not rigorously obeyed in the solid. All the unobserved frequencies were estimated by comparison with $B_3O_3(OH)_3$, $B_3O_3(OD)_3$ from Parsons[7] and $B_3O_3H_3$ and $B_3O_3D_3$ from Gupta and Porter[8] and Lee, Bauer and Wiberley.[9] The D$_{3h}$ assumed symmetry has 14 vibrations of the type $3A_1'$, $2A_2'$, $5E'$, $2A_2''$ and $2E''$ which are given in order above. The B–F bond distance was assumed to be the same as that in BF$_3$. The B–O bond distance was estimated by comparison with other related compounds. The principal moments of inertia are: $I_A = I_B = 45.8345 \times 10^{-39}$, and $I_C = 91.6691 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] D. L. Hildenbrand, L. P. Theard and A. M. Saul, J. Chem. Phys. 39, 1973 (1963).
[2] H. D. Fisher, J. Kiehl and A. Cane, Report HTC-61-90, June 1961, Hughes Tool Company, Culver City, California.
[3] D. D. Smith and R. W. Lawrence, Aerojet Report No. 1952, February 1961, Aerojet-General Corporation.
[4] M. Farber, J. Chem. Phys. 36, 661 (1962). The first $\Delta_r H°$(298.15 K) value was evaluated based on K(1000 K) = 11.8. The second $\Delta_r H°$(298.15 K) values refer to the reaction $B_2O_3(cr) + BF_3(g) = (BOF)_3(g)$.
[5] R. F. Porter, D. R. Bidinosti and K. F. Watterson, J. Chem. Phys. 36, 2104 (1962). The $\Delta_r H°$(298.15 K) value was derived from $\Delta_r H°$(700 K) = 3.46 ± 0.30 kcal·mol^{-1}.
[6] H. D. Fisher, W. J. Lehmann, and I. Shapiro, J. Phys. Chem. 65, 1166 (1961).
[7] J. L. Parsons, J. Chem. Phys. 33, 1860 (1960).
[8] S. K. Gupta and R. F. Porter, J. Phys. Chem. 67, 1286 (1963).
[9] G. H. Lee, W. H. Bauer, and S. E. Wiberley, J. Phys. Chem. 67, 1742 (1963).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K$_f$
0	0.	0.	INFINITE	−21.691	−2357.002	−2357.002	INFINITE
100	57.998	251.201	426.907	−17.571	−2361.671	−2335.147	1219.756
200	89.987	301.683	352.202	−10.104	−2363.963	−2307.608	602.685
250	103.398	323.231	344.283	−5.263	−2364.676	−2293.432	479.187
298.15	115.012	342.454	342.454	0.	−2365.215	−2279.660	399.387
300	115.435	343.167	342.456	0.213	−2365.234	−2279.129	396.832
350	126.216	361.786	343.902	6.260	−2365.667	−2264 743	337.994
400	135.793	379.278	347.242	12.815	−2366.005	−2250.301	293.859
450	144.217	395.770	351.726	19.820	−2366.260	−2235.822	259.527
500	151.566	411.354	356.917	27.218	−2366.431	−2221.318	232.060
600	163.450	440.091	368.427	42.998	−2366.545	−2192.281	190.855
700	172.330	465.987	380.546	59.809	−2366.409	−2163.244	161.423
800	178.998	489.454	392.716	77.391	−2366.095	−2134.241	139.352
900	184.064	510.843	404.671	95.555	−2365.665	−2105.284	122.187
1000	187.969	530.447	416.282	114.165	−2365.170	−2076.379	108.459
1100	191.023	548.511	427.492	133.120	−2364.647	−2047.524	97.229
1200	193.448	565.240	438.283	152.349	−2364.128	−2018.718	87.873
1300	195.399	580.804	448.655	171.794	−2363.636	−1989.954	79.957
1400	196.988	595.345	458.619	191.416	−2363.189	−1961.227	73.174
1500	198.299	608.982	468.193	211.183	−2362.803	−1932.529	67.297
1600	199.390	621.815	477.397	231.069	−2362.490	−1903.855	62.154
1700	200.307	633.932	486.252	251.055	−2362.258	−1875.197	57.618
1800	201.086	645.404	494.778	271.126	−2362.115	−1846.552	53.586
1900	201.751	656.294	502.995	291.268	−2362 064	−1817.911	49.978
2000	202.325	666.657	510.921	311.473	−2362.107	−1789.271	46.731
2100	202.822	676.541	518.574	331.731	−2362.246	−1760.626	43.793
2200	203.255	685.987	525.971	352.035	−2362 479	−1731.972	41.122
2300	203.636	695.030	533.126	372.380	−2362.805	−1703.306	38.683
2400	203.972	703.704	540.054	392.761	−2513.999	−1671.417	36.377
2500	204.269	712.037	546.768	413.173	−2514.735	−1636.294	34.189
2600	204.534	720.054	553.279	433.613	−2515.458	−1601.143	32.167
2700	204 771	727.777	559.600	454.079	−2516.163	−1565.963	30.295
2800	204.983	735.228	565.740	474.567	−2516.848	−1530.757	28.557
2900	205.175	742.425	571.709	495.075	−2517.510	−1495.529	26.937
3000	205.348	749.384	577.517	515.601	−2518.146	−1460.277	25.426
3100	205.505	756.120	583.170	536.144	−2518.753	−1425.004	24.011
3200	205.647	762.646	588.677	556.702	−2519.330	−1389.713	22.685
3300	205.778	768.976	594 045	577.273	−2519.874	−1354.405	21.438
3400	205.897	775.121	599.281	597.857	−2520.383	−1319.079	20.265
3500	206.006	781.091	604.391	618.452	−2520.857	−1283.740	19.159
3600	206.106	786.896	609.380	639.058	−2521.293	−1248.387	18.114
3700	206.199	792.545	614.255	659.673	−2521.690	−1213.024	17.125
3800	206.284	798 045	619.019	680.297	−2522.050	−1177.648	16.188
3900	206.363	803.404	623.678	700.930	−2522.370	−1142.264	15.299
4000	206.436	808.630	628.237	721.570	−2522.652	−1106.874	14.454
4100	206.504	813.728	632.699	742.217	−2522.895	−1071.477	13.651
4200	206.568	818.705	637.069	762.870	−3962.649	−1015.001	12.623
4300	206.627	823.566	641.350	783.530	−3959.555	−944.855	11.478
4400	206.682	828.317	645.545	804.195	−3956.430	−874.783	10.385
4500	206.733	832.962	649.659	824.866	−3953.276	−804.781	9.342
4600	206.781	837.507	653.693	845.542	−3950.095	−734.850	8.344
4700	206.826	841.954	657.652	866.222	−3946 890	−664.987	7.391
4800	206.869	846.309	661.537	886.907	−3943.662	−595.194	6.477
4900	206.908	850.575	665.351	907.596	−3940.414	−525.467	5.602
5000	206.946	854.756	669.098	928.289	−3937.150	−455.807	4.762
5100	206.981	858.854	672.778	948.985	−3933.872	−386.212	3.956
5200	207.014	862.873	676.396	969.685	−3930.583	−316.684	3.181
5300	207.046	866.817	679.951	990.388	−3927.286	−247.216	2.436
5400	207.076	870.687	683.448	1011.094	−3923.986	−177.812	1.720
5500	207.104	874.487	686.887	1031.803	−3920.684	−108.470	1.030
5600	207.130	878.219	690.270	1052.515	−3917.386	−39.185	0.366
5700	207.156	881.886	693.600	1073.229	−3914.094	30.038	−0.275
5800	207.180	885.489	696.877	1093.946	−3910.813	99.206	−0.893
5900	207.202	889.030	700.104	1114.665	−3907.545	168.314	−1.490
6000	207.224	892.513	703.282	1135.386	−3904.296	237.370	−2.066

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

Boroxin ($B_3O_3H_3$) CRYSTAL $M_r = 83.45202$ Boroxin ($B_3H_3O_3$) $B_3H_3O_3$(cr)

$\Delta_f H°(0\ K)$ = Unknown
$S°(298.15\ K) = [167 \pm 42]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_f H°(298.15\ K) = -1262.3 \pm 42\ kJ{\cdot}mol^{-1}$
T_{fus} = Unknown $\Delta_m H°$ = Unknown

Enthalpy of Formation

The value of $\Delta_f H°(298.15\ K)$ for $B_3O_3H_3$(cr) is calculated from the $\Delta_f H°(298.15\ K)$ for $B_3O_3H_3$(g) and $\Delta_{sub} H°(298.15\ K)$ for $B_3O_3H_3$(cr) reported by Porter and Gupta.[1]

Heat Capacity and Entropy

The heat capacities were estimated from those from B_2O_3(cr) and 1/2 B_2H_6Kubaschewski and Evans.[2] The value of $S°(298.15\ K)$ for $B_3O_3H_3$(cr) is calculated based on $\Delta_r S°(298.15\ K) = 6.6\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ for the reaction $B_3O_3H_3(cr) = B_2O_3(am) + 1/2\ B_2H_6(g)$, which was obtained from the calculated $\Delta_r H°(298.15\ K)$ and measured $\Delta_r G°(298.15\ K)$ evaluated from the vapor pressure reported by Sholette and Porter.[3]

Sublimation Data

$\Delta_{sub} H°(298.15\ K)$ is taken from Porter and Gupta.[1]

References

[1] R. F. Porter and S. K. Gupta, J. Phys. Chem. 68, 280 (1964).
[2] O. Kubaschewski and E. Ll. Evans, "Metallurgical Thermochemistry," 3rd ed., Pergamon Press, New York, 426 pp. (1958).
[3] W. P. Sholette and R. F. Porter, J. Phys. Chem. 67, 177 (1963).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	98.324	167.360	167.360	0.	−1262.313	−1156.803	202.667
300	98.742	167.969	167.362	0.182	−1262.355	−1156.148	201.303
400	120.081	199.288	171 488	11.120	−1264.321	−1120.431	146.313
500	141.838	228.436	179.991	24.223	−1265.383	−1084.312	113.277
600	162.758	256.203	190.396	39.484	−1265.199	−1048.093	91.245
700	179.912	282.612	201.700	56 638	−1263.798	−1012.004	75.517
800	194.556	307.628	213.392	75.389	−1261.331	−976.191	63.739
900	205.591	331.204	225.186	95.416	−1258.019	−940.740	54.599
1000	214.221	353.333	236 906	116.427	−1254.093	−905.692	47.309
1100	219.730	374.016	248.442	138.132	−1249.799	−871.057	41.363
1200	224.262	393.337	259.720	160.340	−1245.299	−836.824	36.426
1300	226.786	411.389	270.701	182.895	−1240.725	−802.970	32.264
1400	229.022	428.279	281.360	205.688	−1236.168	−769.467	28.709
1500	230.970	444.148	291.688	228.690	−1231.642	−736.290	25.640
1600	232.630	459.109	301.689	251.872	−1227.166	−703.413	22.964
1700	234.003	473.255	311.369	275.206	−1222.759	−670.814	20.612
1800	235.088	486.662	320.738	298.663	−1218.440	−638.472	18.528
1900	235.886	499.396	329.809	322.214	−1214.232	−606.367	16.670
2000	236.396	511.509	338.594	345.831	−1210.157	−574.479	15.004

PREVIOUS: CURRENT: March 1965

Boroxin ($B_3O_3H_3$) IDEAL GAS $M_r = 83.45202$

$S°(298.15\ K) = [291.91]\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = -1205 \pm 42\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -1218 \pm 42\ kJ \cdot mol^{-1}$

Vibrational Frequencies and Degeneracies υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}
2530 (1)	2620 (2)	903 (1)
[920] (1)	1404 (2)	[300] (1)
[735] (1)	1335 (2)	1115 (2)
[1560] (1)	940 (2)	[230] (2)
[550] (1)	[400] (2)	

Ground State Quantum Weight: [1] $\sigma = [6]$
Point Group: [D_{3h}]
Bond Distances: B–O = [1.36] Å; B–H = [1.18] Å
Bond Angles: B–O–B = [120]°; O–B–H = [120]°
Product of the Moments of Inertia: $I_A I_B I_C = [5.454021 \times 10^{-114}]\ g^3 \cdot cm^6$

Enthalpy of Formation

The equilibrium constants (1290–1481 K) for the reaction (1) 3/2 $H_2(g) + B(am) + B_2O_3(l) = B_3O_3H_3(g)$ were determined by Sholette and Porter.[1] The equilibrium pressures of $B_2H_6(g)$ and $B_3O_3H_3(g)$ for the reaction (2) $B_3O_3H_3(g) = 1/2\ B_2H_6(g) + B_2O_3(cr)$ were measured at 300 K by Porter and Gupta.[2] The equilibrium constants (1246–1326 K) for the reaction[3] $2B_3O_3FH_2(g) = B_3O_3H_3(g) + B_3O_3F_2H(g)$ were reported by Porter and Sholette.[3] Using these data the corresponding enthalpy changes were evaluated by both the 2nd and 3rd law methods.

Reaction	$\Delta_r H°(298.15\ K)$, $kcal \cdot mol^{-1}$ 3rd law	2nd law	$\Delta_f H°(298.15\ K)$ $kcal \cdot mol^{-1}$
(1)	−5.90	+6.52 ± 4.5	−304.0 ± 5.0
(2)**	−11.11	—	−287.6 ± 2.0
	−12.21	—	−272.5 ± 2.0
(3)	−2.0	—	−314 ± 12.0

**The initial system for the first set of measurements was $B_2H_6(g) + B(OH)_3(cr)$. That for the second set was $B_2H_6(g) + B_2O_3(gl)$.

The value of $\Delta_f H°(298.15\ K)$ for $B_3O_3H_3(g)$ adopted is a weighted average of these $\Delta_f H°(298.15\ K)$ values listed.

Heat Capacity and Entropy

The infrared spectrum os solid boroxin has been determined by Gupta and Porter[4] and a partial assignment was made. The infrared spectra of the gas has also been reported by Lee, Bauer, and Wiberley[5] and is in essential agreement with the solid. The assignment of the frequencies has been changed slightly due to the non–appearance of the band at 1115 cm^{-1} in the gas phase. The assumed D_{3h} symmetry has 14 vibrations of the type $3A_1'$, $2A_2'$, $5E'$, $2A_2''$, and $2E''$, and 7 estimated frequencies were obtained by comparison with $B_3O_6H_3$, by Parsons.[6]

The point group, bond angles and bond lengths were assumed to be the same as for $(BOF)_3(g)$. The B–H bond length was taken as the sum of the single covalent radii of the atoms. The principal moments of inertia are: $I_A = I_B = 13.9710 \times 10^{-39}$, and $I_C = 27.9421 \times 10^{-39}\ g \cdot cm^2$.

References

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Boroxin ($B_3H_3O_3$) $B_3H_3O_3(g)$

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ $J \cdot K^{-1} mol^{-1}$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$ $kJ \cdot mol^{-1}$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−16.846	−1205.022	−1205.022	INFINITE
100	44.531	223.177	355.472	−13.230	−1210.334	−1191.454	622.352
200	67.194	261.217	299.274	−7.612	−1214.122	−1171.045	305.846
250	77.761	277.347	293.296	−3.987	−1215.892	−1160.070	242.383
298.15	87.831	291.907	291.907	0.	−1217.544	−1149.168	201.329
300	88.213	292.451	291.909	0.163	−1217.606	−1148.743	200.014
350	98.298	306.813	293.020	4.828	−1219.211	−1137.138	169.708
400	107.750	320.564	295.609	9.982	−1220.690	−1125.310	146.950
450	116.426	333.765	299.120	15.590	−1222.032	−1113.306	129.229
500	124.290	346.445	303.223	21.611	−1223.226	−1101.160	115.037
600	137.736	370.338	312.444	34.736	−1225.177	−1076.554	93.722
700	148.586	392.415	322.312	49.072	−1226.596	−1051.664	78.476
800	157.375	412.850	332.369	64.385	−1227.565	−1026.603	67.030
900	164.538	431.814	342.377	80.493	−1228.173	−1001.443	58.122
1000	170.415	449.464	352.214	97.250	−1228.501	−976.231	50.993
1100	175.270	465.941	361.812	114.542	−1228.621	−950.996	45.159
1200	179.307	481.370	371.139	132.277	−1228.594	−925.758	40.297
1300	182.687	495.859	380.182	150.381	−1228.469	−900.526	36.184
1400	185.535	509.505	388.936	168.796	−1228.290	−875.306	32.658
1500	187.952	522.390	397.408	187.474	−1228.089	−850.100	29.603
1600	190.014	534.588	405.604	206.375	−1227.895	−824.908	26.930
1700	191.786	546.162	413.534	225.467	−1227.729	−799.726	24.573
1800	193.316	557.169	421.211	244.724	−1227.611	−774.553	22.477
1900	194.646	567.657	428.645	264.124	−1227.554	−749.385	20.602
2000	195.807	577.671	435.848	283.648	−1227.571	−724.218	18.915
2100	196.826	587.250	442.831	303.280	−1227.673	−699.048	17.388
2200	197.725	596.428	449.605	323.009	−1227.866	−673.871	16.000
2300	198.521	605.235	456.182	342.822	−1228.157	−648.684	14.732
2400	199.228	613.699	462.570	362.710	−1379.331	−620.275	13.500
2500	199.860	621.845	468.779	382.665	−1380.068	−588.633	12.299
2600	200.427	629.695	474.818	402.680	−1380.819	−556.961	11.189
2700	200.936	637.269	480.695	422.748	−1381.588	−525.259	10.162
2800	201.396	644.585	486.418	442.865	−1382.377	−493.528	9.207
2900	201.812	651.659	491.995	463.026	−1383.188	−461.770	8.317
3000	202.190	658.507	497.432	483.227	−1384.024	−429.983	7.487
3100	202.534	665.143	502.735	503.463	−1384.886	−398.167	6.709
3200	202.848	671.578	507.912	523.732	−1385.775	−366.324	5.980
3300	203.136	677.825	512.966	544.032	−1386.692	−334.452	5.294
3400	203.399	683.893	517.905	564.359	−1387.639	−302.551	4.648
3500	203.642	689.792	522.732	584.711	−1388.614	−270.623	4.039
3600	203.865	695.532	527.453	605.086	−1389.620	−238.666	3.463
3700	204.071	701.121	532.071	625.483	−1390.656	−206.682	2.918
3800	204.262	706.566	536.592	645.900	−1391.723	−174.667	2.401
3900	204.439	711.874	541.019	666.335	−1392.821	−142.624	1.910
4000	204.604	717.052	545.355	686.788	−1393.951	−110.555	1.444
4100	204.756	722.106	549.605	707.256	−1395.112	−78.455	1.000
4200	204.899	727.042	553.771	727.739	−2835.853	−25.255	0.314
4300	205.032	731.865	557.857	748.235	−2833.817	41.641	−0.506
4400	205.156	736.580	561.865	768.745	−2831.818	108.488	−1.288
4500	205.272	741.192	565.799	789.266	−2829.858	175.290	−2.035
4600	205.381	745.704	569.661	809.799	−2827.938	242.049	−2.749
4700	205.484	750.122	573.454	830.342	−2826.059	308.768	−3.432
4800	205.580	754.450	577.180	850.895	−2824.222	375.448	−4.086
4900	205.670	758.689	580.841	871.458	−2822.428	442.089	−4.713
5000	205.755	762.845	584.440	892.029	−2820.679	508.695	−5.314
5100	205.836	766.921	587.978	912.609	−2818.975	575.265	−5.892
5200	205.912	770.918	591.458	933.196	−2817.319	641.801	−6.447
5300	205.983	774.841	594.881	953.791	−2815.711	708.309	−6.981
5400	206.051	778.692	598.249	974.393	−2814.154	774.784	−7.495
5500	206.115	782.474	601.564	995.001	−2812.647	841.231	−7.989
5600	206.176	786.188	604.828	1015.616	−2811.193	907.654	−8.466
5700	206.234	789.838	608.042	1036.236	−2809.794	974.049	−8.926
5800	206.289	793.425	611.207	1056.862	−2808.450	1040.422	−9.370
5900	206.341	796.952	614.326	1077.494	−2807.163	1106.767	−9.799
6000	206.391	800.420	617.399	1098.131	−2805.936	1173.096	−10.213

PREVIOUS: March 1965 (1 atm) — CURRENT: March 1965 (1 bar)

Boroxin ($B_3H_3O_3$) $B_3H_3O_3(g)$

Boric Acid ($(HBO_2)_3$) IDEAL GAS $M_r = 131.45022$ Boric Acid ($(HBO_2)_3$) $B_3H_3O_6(g)$

$\Delta_fH°(0\ K) = [-2252 \pm 13]\ kJ{\cdot}mol^{-1}$
$S°(298.15\ K) = [347.57]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298.15\ K) = [-2272 \pm 13]\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}
[550] (1)	[250] (1)	[600] (2)
[1150] (1)	[500] (1)	[450] (2)
[950] (1)	[350] (1)	[3500] (2)
[3500] (1)	[750] (2)	[350] (2)
[1100] (1)	[900] (2)	[200] (2)
[600] (1)	[1300] (2)	[1000] (2)
[500] (1)	[1000] (2)	

Ground State Quantum Weight: 1 $\sigma = 3$
Point Group: C_{3h}
Bond Distances: B–O = [1.36] Å; O–H = [1.1] Å
Bond Angles: H–O–B = [120]°; O–B–O = [120]°; B–O–B = [120]°
Product of the Moments of Inertia: $I_AI_BI_C = [1.776533 \times 10^{-112}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The equilibrium constant, K_f (1451 K) = 0.9 for the reaction $H_3BO_3(l) + B_2O_3(l) = (HBO_2)_3(g)$ was reported by Meschi, Chupka and Berkowitz,[1] which was determined by means of mass spectrometry. The equilibrium constants of the reactions between water vapor and liquid B_2O_3 were determined at 1147 K by Blauer and Farber[2] by use of a transpiration method. From the reported value, $1.5\,K_2 + 0.5\,K_1 = 0.0342 \pm 0.0095$, the equilibrium constant, K_2, for the reaction $1.5\ B_2O_3(l) + 1.5\ H_2O(g) = (HBO_2)_3($ derived as 0.0168, using $K_3 = 0.0181$ for the reaction $0.5\ B_2O_3(l) + 1.5\ H_2O(g) = H_3BO_3(g)$ evaluated by use of JANAF values of $\Delta_fG°$ for $B_2O_3(l)$, $H_2O(g)$ and $H_3BO_3(g)$. Employing the equilibrium constants obtained, the respective enthalpy changes for the two reactions were calculated by the 3rd law method. The corresponding values of $\Delta_fH°(298.15\ K)$ for $(HBO_2)_3(g)$ were also derived.

Source	Chemical Reaction	$\Delta_rH°(298.15\ K)$ kcal·mol^{-1}	$\Delta_fH°(298.15$ kcal·mol^{-1}
Meschi, *et al.*[1]	$H_3BO_3(l) + B_2O_3(l) = (HBO_2)_3(g)$	−7.31	−543.8
Blauer and Farber[2]	$1.5\ B_2O_3(l) + 1.5\ H_2O(g) = (HBO_2)_3(g)$	−6.67	−542.3

The adopted value of $\Delta_fH°(298.15\ K)$ for $(HBO_2)_3(g)$ is the average of these two listed in the above table. The equilibrium constants for the same reactions between $B_2O_3(l)$ and $H_2O(g)$ were also determined by a transpiration method in the temperature region 1000–1273 K by Randall and Margrave.[3] The reported value, $\Delta_fH°(0\ K) = -537.5 \pm 3\ kcal{\cdot}mol^{-1}$ for $(HBO_2)_3(g)$, is in good agreement with the value adopted.

Heat Capacity and Entropy

All the molecular and spectroscopic constants were estimated by White, Mann, Walsh, and Sommer.[4] The principal moments of inertia are: $I_A = 43.6915 \times 10^{-39}$, $I_B = 45.5585 \times 10^{-39}$, and $I_C = 89.2499 \times 10^{-39}\ g{\cdot}cm^2$. The infrared absorption spectra for $B_3O_3(OH)_3(cr)$ in the 430 to 4000 cm^{-1} was reported by Parsons.[5] A partial Raman spectrum was also given.

References

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[5] J. L. Parsons, J. Chem. Phys. 33, 1860 (1960).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−22.763	−2252.282	−2252.282	INFINITE
100	51.541	251.641	441.169	−18.953	−2261.757	−2219.727	1159.467
200	96.849	301.091	358.876	−11.557	−2268.134	−2174.986	568.048
250	118.479	325.060	349.724	−6.166	−2270.324	−2151.434	449.518
298.15	137.265	347.567	347.567	0.	−2271.912	−2128.384	372.884
300	137.941	348.418	347.570	0.255	−2271.964	−2127.493	370.430
350	154.896	370.988	349.313	7.586	−2273.117	−2103.317	313.903
400	169.352	392.642	353.386	15.702	−2273.876	−2079.004	271.490
450	181.535	413.313	358.906	24.483	−2274.320	−2054.616	238.494
500	191.764	432.985	365.338	33.823	−2274.508	−2030.192	212.093
600	207.660	469.433	379.702	53.839	−2274.309	−1981.336	172.491
700	219.256	502.359	394.912	75.213	−2273.571	−1932.560	144.209
800	228.061	532.236	410.239	97.597	−2272.474	−1883.916	123.007
900	235.010	559.514	425.332	120.764	−2271.132	−1835.424	106.525
1000	240.666	584.577	440.020	144.557	−2269.617	−1787.093	93.348
1100	245.378	607.742	454.228	168.866	−2267.983	−1738.918	82.574
1200	249.367	629.269	467.929	193.608	−2266.271	−1690.896	73.603
1300	252.782	649.367	481.121	218.720	−2264.515	−1643.019	66.017
1400	255.730	668.211	493.818	244.149	−2262.741	−1595.278	59.521
1500	258.293	685.944	506.042	269.853	−2260.976	−1547.665	53.894
1600	260.531	702.686	517.813	295.797	−2259.240	−1500.167	48.975
1700	262.495	718.541	529.159	321.950	−2257.550	−1452.777	44.638
1800	264.225	733.595	540.102	348.288	−2255.925	−1405.486	40.786
1900	265.756	747.923	550.666	374.788	−2254.376	−1358.282	37.342
2000	267.115	761.590	560.873	401.433	−2252.917	−1311.156	34.244
2100	268.325	774.652	570.744	428.206	−2251.556	−1264.102	31.443
2200	269.406	787.160	580.299	455.094	−2250.302	−1217.109	28.898
2300	270.376	799.157	589.555	482.084	−2249.163	−1170.173	26.575
2400	271.248	810.683	598.531	509.166	−2398.922	−1120.077	24.378
2500	272.034	821.772	607.240	536.331	−2398.262	−1066.805	22.290
2600	272.745	832.456	615.698	563.570	−2397.633	−1013.560	20.363
2700	273.389	842.761	623.918	590.877	−2397.039	−960.337	18.579
2800	273.975	852.715	631.912	618.246	−2396.482	−907.135	16.923
2900	274.509	862.338	639.693	645.671	−2395.966	−853.955	15.381
3000	274.997	871.653	647.271	673.146	−2395.492	−800.790	13.943
3100	275.444	880.677	654.655	700.669	−2395.062	−747.639	12.598
3200	275.854	889.429	661.856	728.234	−2394.676	−694.505	11.337
3300	276.231	897.923	668.881	755.839	−2394.335	−641.380	10.152
3400	276.578	906.175	675.740	783.479	−2394.038	−588.264	9.038
3500	276.899	914.197	682.439	811.153	−2393.788	−535.157	7.987
3600	277.196	922.002	688.985	838.858	−2393.583	−482.056	6.994
3700	277 471	929.600	695.386	866.592	−2393.424	−428.962	6.056
3800	277.726	937.003	701.648	894.352	−2393.311	−375.867	5.167
3900	277.963	944.220	707.775	922.136	−2393.242	−322.776	4.323
4000	278.184	951.261	713.775	949.944	−2393.220	−269.690	3.522
4100	278.390	958.132	719.651	977.773	−2393.243	−216.601	2.760
4200	278.583	964.843	725.410	1005.621	−3832.860	−142.439	1.771
4300	278.763	971.401	731.054	1033.489	−3829.713	−54.608	0.663
4400	278.931	977.811	736.590	1061.374	−3826.619	33.148	−0.394
4500	279.089	984.081	742.020	1089.275	−3823.576	120.834	−1.403
4600	279.238	990.217	747.349	1117.191	−3820.587	208.453	−2.367
4700	279.378	996.224	752.581	1145.122	−3817.655	296.011	−3.290
4800	279.509	1002.107	757.718	1173.066	−3814.779	383.505	−4.173
4900	279.633	1007.872	762.765	1201.024	−3811.962	470.942	−5.020
5000	279.750	1013.522	767.724	1228.993	−3809.206	558.321	−5.833
5100	279.860	1019.063	772.598	1256.973	−3806.514	645.645	−6.613
5200	279.964	1024.498	777.390	1284.965	−3803.886	732.913	−7.362
5300	280.063	1029.832	782.103	1312.966	−3801.326	820.138	−8.083
5400	280.157	1035.068	786.739	1340.977	−3798.837	907.310	−8.776
5500	280.245	1040.209	791.301	1368.997	−3796.420	994.437	−9.444
5600	280.329	1045.260	795.791	1397.026	−3794.079	1081.525	−10.088
5700	280.409	1050.222	800.211	1425.063	−3791.816	1168.568	−10.709
5800	280.485	1055.100	804.564	1453.108	−3789.635	1255.576	−11.308
5900	280.557	1059.895	808.851	1481.160	−3787.539	1342.538	−11.886
6000	280.626	1064.611	813.075	1509.219	−3785.531	1429.475	−12.445

PREVIOUS: December 1964 (1 atm) CURRENT: December 1964 (1 bar)

Borazine ($B_3N_3H_6$) IDEAL GAS $M_r = 80.49774$ Borazine ($B_3H_6N_3$) $B_3H_6N_3(g)$

$\Delta_fH°(0\ K) = -484.5 \pm 13\ kJ{\cdot}mol^{-1}$

$S°(298.15\ K) = 288.72\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298\ 15\ K) = -510.0 \pm 13\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

υ, cm^{-1}	υ, cm^{-1}
3450 (1)	3400 (2)
[554] (1)	[339] (1)
[266] (1)	528 (1)

Ground State Quantum Weight: 1 $\sigma = 6$
Point Group: D_{3h}
Bond Distances: B–N = 1.44 Å; B–H = 1.20 Å; H–N = 1.02 Å
Bond Angles: N–B–N = 120°; B–N–B = 120°; N–B–H = 120°
Product of the Moments of Inertia: $I_AI_BI_C = 8.326395 \times 10^{-114}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The enthalpy of combustion for the reaction $B_3N_3H_6(l) + 15/4\ O_2(g) + 3/2\ H_2O(l) = 3\ H_3BO_3(c) + 3/2\ N_2(g)$ was reported to be $-552.9 \pm 3.0\ kcal{\cdot}mol^{-1}$ by Kilday, Johnson and Prosen.[1] $\Delta_fH°(H_3BO_3$, cr, 298.15 K) = $-261.47\ kcal{\cdot}mol^{-1}$ from JANAF tables were used to calculate $\Delta_fH°(B_3N_3H_6$, l, 298.15 K) = $-129\ 0 \pm 3.0\ kcal{\cdot}mol^{-1}$. Vapor pressure data on $B_3N_3H_6(l)$ reported by Stock and Pohland[3] were fitted to a linear least squares. ΔC_p(l–g) for borazine was approximated by benzene to calculate a 2nd law $\Delta_{vap}H°$(298.15 K) = $7.1 \pm 0.1\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

The fundamental frequency assignment was made by Crawford and Edsall.[4] The three frequencies enclosed by brackets are calculated values. The principal moments of inertia are calculated from molecular constants given by Bauer.[5] The principal moments of inertia are: $I_A = I_B = 16.0870 \times 10^{-39}$, and $I_C = 32.1740 \times 10^{-39}\ g{\cdot}cm^2$.

References

[1] M. V. Kilday, W H. Johnson, and E. J. Prosen, J. Res. Nat. Bur. Stand. 65A, 101 (1961).
[2] U. S Nat. Bur. Stand. Circ. 500, 1268 pp. (1962).
[3] A. Stock and E. Pohland, Ber. 59, 2215 (1926).
[4] B. L. Crawford, Jr. and J. T. Edsall, J. Chem. Phys. 7, 223 (1939).
[5] S. H. Bauer, J. Am. Chem. Soc 60, 524 (1938).

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−16.515	−484.495	−484.495	INFINITE
100	39.386	222.416	352.981	−13.056	−494.460	−462.420	241.543
200	65.053	256.820	296.554	−7.947	−502.796	−427.066	111.538
250	81.262	273.063	290.231	−4.292	−506.627	−407.685	85.181
298.15	96.927	288.723	288.723	0.	−510.030	−388.315	68.031
300	97.516	289.324	288.725	0.180	−510.154	−387.560	67.480
350	112.826	305.522	289.969	5.444	−513.304	−366.873	54.753
400	126.782	321.515	292.916	11.440	−516.075	−345.761	45.152
450	139.307	337.185	296.967	18.098	−518.480	−324.323	37.646
500	150.485	352.452	301.756	25.348	−520.537	−302.637	31.616
600	169.391	381.623	312.662	41.377	−523.714	−258.739	22.525
700	184.667	408.922	324.486	59.105	−525.828	−214.396	15.998
800	197.230	434.427	336.652	78.220	−527.084	−169.811	11.088
900	207.712	458.281	348.856	98.482	−527.656	−125.111	7.261
1000	216.552	480.636	360.928	119.708	−527.689	−80.378	4.198
1100	224.064	501.637	372.775	141.748	−527.300	−35.662	1.693
1200	230.486	521.416	384.346	164.484	−526.590	9.003	−0.392
1300	236.003	540.088	395.614	187.815	−525.636	53.598	−2.154
1400	240.763	557.756	406.571	211.659	−524.504	98.113	−3.661
1500	244.887	574.511	417.213	235.947	−523.246	142.543	−4.964
1600	248.475	590.433	427.546	260.619	−521.905	186.885	−6.101
1700	251.610	605.593	437.577	285.627	−520.514	231.142	−7.102
1800	254.359	620.054	447.316	310.928	−519.102	275.316	−7.989
1900	256.779	633.872	456.774	336.488	−517.691	319.412	−8.781
2000	258.918	647.099	465.962	362.274	−516.299	363.434	−9.492
2100	260.815	659.778	474.891	388.263	−514.942	407.387	−10.133
2200	262.503	671.951	483.574	414.430	−513.632	451.277	−10.715
2300	264.011	683.654	492.020	440.758	−512.379	495.108	−11.244
2400	265.363	694.919	500.241	467.228	−661.971	542.093	−11.798
2500	266.579	705.777	508.247	493.826	−661.093	592.244	−12.374
2600	267.675	716.254	516.047	520.539	−660.198	642.360	−12.905
2700	268.666	726.375	523.650	547.357	−659.291	692.441	−13.396
2800	269.565	736.162	531.066	574.269	−658.378	742.488	−13.851
2900	270.382	745.636	538.303	601.267	−657.465	792.503	−14.275
3000	271.128	754.815	545.367	628.343	−656.555	842.487	−14.669
3100	271.809	763.717	552.268	655.491	−655.652	892.439	−15.038
3200	272.433	772.356	559.012	682.703	−654.759	942.364	−15.383
3300	273.006	780.748	565.604	709.976	−653.880	992.261	−15.706
3400	273.534	788.906	572.053	737.303	−653.018	1042.130	−16.010
3500	274.020	796.843	578.362	764.681	−652.174	1091.975	−16.297
3600	274.469	804.568	584.539	792.106	−651.351	1141.796	−16.567
3700	274.885	812.094	590.588	819.574	−650.551	1191.595	−16.822
3800	275.270	819.430	596.514	847.082	−649.777	1241.373	−17.064
3900	275.628	826.585	602.322	874.627	−649.030	1291.130	−17.293
4000	275.961	833.568	608.016	902.207	−648.311	1340.868	−17.510
4100	276.272	840.386	613.601	929.818	−647.623	1390.589	−17.716
4200	276.561	847.047	619.080	957.460	−2086.514	1461.366	−18.175
4300	276.832	853.558	624.458	985.130	−2082.627	1545.794	−18.778
4400	277.086	859.925	629.737	1012.826	−2078.778	1630.131	−19.352
4500	277.323	866.154	634.922	1040.547	−2074.970	1714.381	−19.900
4600	277.546	872.252	640.015	1068.290	−2071.202	1798.547	−20.423
4700	277.756	878.223	645.020	1096.055	−2067.477	1882.632	−20.923
4800	277.953	884.073	649.940	1123.841	−2063.794	1966.639	−21.401
4900	278.138	889.806	654.776	1151.646	−2060.155	2050.567	−21.859
5000	278.313	895.427	659.533	1179.468	−2056.561	2134.424	−22.298
5100	278.478	900.940	664.213	1207.308	−2053.011	2218.207	−22.719
5200	278.635	906.349	668.818	1235.164	−2049.505	2301.923	−23.123
5300	278.782	911.658	673.350	1263.035	−2046.044	2385.571	−23.511
5400	278.922	916.870	677.811	1290.920	−2042.627	2469.155	−23.884
5500	279.055	921.990	682.204	1318.819	−2039.254	2552.674	−24.243
5600	279.180	927.019	686.531	1346.730	−2035.924	2636.134	−24.589
5700	279.299	931.961	690.794	1374.655	−2032.637	2719.535	−24.922
5800	279.413	936.820	694.994	1402.590	−2029.392	2802.878	−25.243
5900	279.521	941.597	699.133	1430.537	−2026.189	2886.164	−25.552
6000	279.623	946.296	703.214	1458.494	−2023.026	2969.398	−25.851

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

Potassium Borate ($K_2B_4O_7$) CRYSTAL $M_r = 233.4324$ Potassium Borate ($K_2B_4O_7$) $B_4K_2O_7(cr)$

$S°(298.15\ K) = [208.4 \pm 6.3]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 1088\ K$

$\Delta_fH°(0\ K) =$ Unknown
$\Delta_fH°(298.15\ K) = -3334.2\ kJ{\cdot}mol^{-1}$
$\Delta_{fus}H° = 104.5 \pm 4.2\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

$\Delta_fH°(298.15\ K)$ was recalculated from the experimental data of Shartsis and Capps.[1] They studied the enthalpy of solution of various alkali borates in 2N nitric acid. Average molecular weights were used for physical mixtures of the oxides B_2O_3 and R_2O (where R is either Li, Na, or K) rather than for the borate compounds $R_2O{\cdot}nB_2O_3$ present. These incorrect molecular weights led to spurious correlations and faulty conclusions. In reinterpreting the data, the steps followed were: (1) The calculation of the correct molecular weights and molar enthalpies of reaction; (2) The establishment that the enthalpy of formation of the borates from the oxides is linear with the mole fraction of B_2O_3 in the total original moles of oxides for the reactions

$$R_2O(cr) + nB_2O_3(gl) \rightarrow R_2O{\cdot}nB_2O_3(gls) \quad (I)$$
$$\text{and } R_2O(cr) + nB_2O_3(gl) \rightarrow R_2O{\cdot}nB_2O_3(cr) \quad (II)$$

With the enthalpy of formation being zero at 100 percent R_2O; (3) The evaluation of the least square fit of the line through the enthalpy of reaction data for reaction I and for reaction II. (4) The use of the proper weighting factors in applying least squares to adjust for both the sample size and the molecular weight of the mixture of borates used in each solution experiment.

Heat Capacity and Entropy

The enthalpy measurements of Smith,[2] in the range 298–973 K were smoothed graphically and were used to obtain a smooth set of C_p data. The heat capacity was extrapolated smoothly above this region. The entropy at 298.15 K is estimated from that of $Na_2B_4O_7(cr)$ by using an average entropy change of $4.5 \pm 1.5\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ on substituting Na_2 by K_2.

Fusion Data

T_{fus} was given by Rollet.[3] The enthalpy of melting was obtained from the enthalpies of formation of the crystal and glass at 298.15 K combined with the enthalpy differences between 298.15 K and 1088 K. This involves a slight extrapolation of the crystal data and an uncertainty of about $1.0\ kcal{\cdot}mol^{-1}$.

References

[1] L. Shartsis and W. Capps, J. Am. Ceram. Soc. 37, 27 (1954).
[2] *G. S. Smith, Ph. D. Thesis, Penn. State Univ.*, Univ. Microfilms, Order No. Mic 59–2916 (1959).
[3] A. P. Rollet, Comp. Rend. 200, 1763 (1935).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	$\log K_f$
0							
90							
200							
250							
298.15	170.498	208.363	208.363	0.	−3334.230	−3136.756	549.547
300	171.335	209.420	208.366	0.316	−3334.297	−3135.531	545.944
400	206.271	263.696	215.530	19.267	−3342.152	−3067.880	400.624
500	232.798	312.737	230.150	41.293	−3343.971	−2999.075	313.311
600	250.538	356.839	247.657	65.509	−3344.817	−2930.004	255.080
700	262.379	396.388	266.130	91.181	−3345.149	−2860.838	213.478
800	271.123	432.022	284.677	117.876	−3345.218	−2791.644	182.276
900	277.399	464.322	302.871	145.306	−3345.200	−2722.448	158.007
1000	283.257	493.860	320.514	173.346	−3345.151	−2653.256	138.592
1088.000	287.723	517.940	335.520	198.474	--- CRYSTAL <--> LIQUID ---		
1100	288.282	521.099	337.527	201.930	−3503.006	−2574.848	122.269
1200	292.478	546.369	353.890	230.975	−3500.895	−2490.563	108.411
1300	295.842	569.918	369.612	260.398	−3498.737	−2406.456	96.693
1400	298.374	591.940	384.715	290.115	−3496.583	−2322.515	86.654
1500	300.076	612.589	399.226	320.045	−3494.495	−2238.727	77.959

PREVIOUS: CURRENT: March 1963

Potassium Borate ($K_2B_4O_7$) $B_4K_2O_7(cr)$

Potassium Borate ($K_2B_4O_7$) LIQUID M_r = 233.4324 Potassium Borate ($K_2B_4O_7$) $B_4K_2O_7(l)$

S°(298.15 K) = [237.120] J·K^{-1}·mol^{-1}
T_{fus} = 1088 K

$\Delta_f H^\circ$(298.15 K) = [−3289.042] kJ·mol^{-1}
$\Delta_{fus} H^\circ$ = 104.5 ± 4.2 kJ·mol^{-1}

Enthalpy of Formation

The enthalpy of formation is obtained form reaction (1), as given on the crystal table.

Heat Capacity and Entropy

The enthalpy measurements of Smith[1] in the range 298 to 1373 K on the glass and liquid were smoothed graphically and used to determine C_p. There is a discontinuity (glass transition) in the C_p curve at 676 K. Above 1373 K the C_p values were extrapolated smoothly.

The entropy at 298.15 K is calculated from that of the crystal by adding $\Delta_{fus}S^\circ$ and the entropy differences, S°(1088 K)–S°(298.15 K), between the crystal and liquid.

Fusion Data

Refer to the crystal table for details.

Reference

[1] G. S. Smith, Ph. D. Thesis, Penn. State Univ., Univ. Microfilms, Order No. Mic 59–2916 (1959).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0							
100							
200							
250							
298.15	170.498	237.120	237.120	0.	−3289.042	−3100.143	543.132
300	171.335	238.177	237.124	0.316	−3289.110	−3098.971	539.579
400	206.271	292.453	244.287	19.266	−3296.965	−3034.195	396.225
500	232.840	341.499	258.908	41.296	−3298.781	−2968.266	310.093
600	250.538	385.610	276.416	65.516	−3299.623	−2902.072	252.648
676.000	259.821	416.068	290.428	84.933	GLASS <--> LIQUID TRANSITION		
676.000	369.237	416.068	290.428	84.933			
700	375.221	429.053	294.959	93.866	−3297.277	−2835.830	211.612
800	402.501	480.977	315.000	132.781	−3285.126	−2770.715	180.909
900	426.266	529.790	336.181	174.249	−3271.070	−2707.239	157.124
1000	446.558	575.818	357.866	217.952	−3255.357	−2645.420	138.183
1088.000	457.879	613.958	377.052	257.753	--- CRYSTAL <--> LIQUID ---		
1100	459.361	618.988	379 664	263.257	−3396.492	−2576.011	122.325
1200	471.143	659.470	401.312	309.790	−3376.892	−2502.281	108.921
1300	481.913	697.614	422.651	357.452	−3356.496	−2430.219	97.647
1400	491.670	733.691	443.591	406.139	−3335.372	−2359.755	88.044
1500	500.406	767.916	464.082	455.752	−3313.601	−2290.825	79.774
1600	507.268	800.434	484.096	506.140	−3291.314	−2223.364	72.585
1700	513.544	831.378	503.622	557.186	−3268.619	−2157.310	66.286
1800	519.234	860.896	522.657	608.830	−3245.569	−2092.603	60.726
1900	524.339	888.108	541.207	661.013	−3222.218	−2029.185	55.786
2000	528.858	916.121	559.282	713.678	−3198.621	−1967.003	51.373
2100	532.188	942.006	576.895	766.732	−3174.868	−1906.006	47.409
2200	535.234	966.835	594.059	820.106	−3151.032	−1846.140	43.833
2300	537.995	990.689	610.789	873.770	−3127.143	−1787.363	40.592
2400	540.472	1013.639	627.099	927.696	−3304.266	−1725.350	37.551
2500	542.665	1035.747	643.005	981.855	−3280.672	−1660.046	34.685
2600	544.573	1057.069	658.523	1036.219	−3256.986	−1595.688	32.058
2700	546.196	1077.653	673.668	1090.760	−3233.240	−1532.242	29.643
2800	547.535	1097.542	688.453	1145.449	−3209.468	−1469.676	27.417
2900	548.589	1116.775	702.893	1200.257	−3185.701	−1407.963	25.360
3000	549.359	1135.387	717.001	1255.157	−3161.975	−1347.065	23.454

PREVIOUS: CURRENT: March 1963

Potassium Borate ($K_2B_4O_7$) CRYSTAL-LIQUID

298.15	to 1088 K	crystal
above	1088 K	liquid

Refer to the individual tables for details.

M_r = 233.4324 Potassium Borate ($K_2B_4O_7$) $B_4K_2O_7(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0							
100							
200							
250							
298.15	170.498	208.363	208.363	0.	−3334.230	−3136.756	549.547
300	171.335	209.420	208.366	0.316	−3334.297	−3135.531	545.944
400	206.271	263.696	215.530	19.267	−3342.152	−3067.880	400.624
500	232.798	312.737	230.150	41.293	−3343.971	−2999.075	313.311
600	250.538	356.839	247.657	65.509	−3344.817	−2930.004	255.080
700	262.379	396.388	266.130	91.181	−3345.149	−2860.838	213.478
800	271.123	432.022	284 677	117.876	−3345.218	−2791.644	182.276
900	277.399	464.322	302.871	145.306	−3345.200	−2722.448	158.007
1000	283.257	493.860	320.514	173.346	−3345.151	−2653.256	138.592
1088.000	287.723	517.940	335.520	198.474	____ CRYSTAL <--> LIQUID ____		
1088.000	457.879	613.958	335.520	302.940	TRANSITION		
1100	459.361	618.988	338.585	308.444	−3396.492	−2576.011	122.325
1200	471.143	659.470	363.656	354.978	−3376.892	−2502.281	108.921
1300	481.913	697.614	387.892	402.639	−3356.496	−2430.219	97.647
1400	491.670	733.691	411.315	451.327	−3335.372	−2359.755	88.044
1500	500.406	767.916	433.957	500.939	−3313.601	−2290.825	79.774
1600	507.268	800.434	455.854	551.327	−3291.314	−2223.364	72.585
1700	513.544	831.378	477.041	602.373	−3268.619	−2157.310	66.286
1800	519.234	860.896	497.553	654.017	−3245.569	−2092.603	60.726
1900	524.339	889.108	517.424	706.200	−3222.218	−2029.185	55.786
2000	528.858	916.121	536.688	758.865	−3198.621	−1967.003	51.373
2100	532.188	942.006	555.377	811.920	−3174.868	−1906.006	47.409
2200	535.234	966.835	573.519	865.293	−3151.033	−1846.140	43.833
2300	537.995	990.689	591.142	918.957	−3127.143	−1787.363	40.592
2400	540.472	1013.639	608.271	972.883	−3304.266	−1725.350	37.551
2500	542.665	1035.747	624.931	1027.042	−3280.672	−1660.046	34.685
2600	544.573	1057.069	641.144	1081.406	−3256.986	−1595.688	32.058
2700	546.196	1077.653	656.932	1135.947	−3233.240	−1532.242	29.643
2800	547.535	1097.542	672.315	1190.636	−3209.468	−1469.676	27.417
2900	548.589	1116.775	687.311	1245.445	−3185.701	−1407.963	25.360
3000	549.359	1135.387	701.938	1300.344	−3161.975	−1347.065	23.454

PREVIOUS. CURRENT: March 1963

Lithium Borate ($Li_2B_4O_7$) CRYSTAL M_r = 169.1178

$\Delta_f H°$(0 K) = Unknown

$S°$(298 15 K) = [155 6 ± 4.2] J K^{-1}·mol^{-1} $\Delta_f H°$(298 15 K) = −3362 3 ± 6 3 kJ·mol^{-1}

T_{fus} = 1190 ± 2 K $\Delta_{fus}H°$ = 120.5 ± 6 3 kJ·mol^{-1}

Enthalpy of Formation

The enthalpy of formation was calculated from $\Delta_r H°$(298.15 K) = −12 2 kcal for the reaction $Li_2B_4O_7$(cr) + 2 HNO_3(aq) + 5 H_2O(l) = 4 H_3BO_3(aq) + 2 $LiNO_3$(aq). Capps[1] Auxilliary data are from National Bureau of Standards Circular 500.[2]

Heat Capacity and Entropy

The enthalpy measurements of Smith[3] in the range 298 to 1190 K were smoothed graphically and used to determine C_p. A linear extrapolation of C_p was used from 1190 to 2000 K.

$S°$(298.15 K) was estimated by three routes: (1) $S°$($Li_2B_4O_7$, cr, 298.15 K) = 37.3 cal K^{-1}·mol^{-1} based on JANAF $S°$($Na_2B_4O_7$, cr, 298 15 K) = 45 3 and $\Delta S°$(2Na–2Li, 298.15 K) = 8 cal·K^{-1}·mol^{-1} from Latimer;[4] (2) $S°$($Li_2B_4O_7$, cr, 298.15 K) = 36.7 cal K^{-1}·mol^{-1} in a similar manner based on $\Delta_f S°$(2Na$^+$–2Li$^+$, 298.15 K) = 8.6 cal·K^{-1}·mol^{-1} from Kelley,[5] and (3) $S°$($Li_2B_4O_7$, cr, 298.15 K) = 37.6 cal·K^{-1}·mol^{-1} based on addition of the JANAF entropies for 2$LiBO_2$ and B_2O_3. The value adopted is an average of these estimates.

Fusion Data

The value for T_{fus} is from Sastry and Hummel.[6] Rollet and Bouaziz[7] earlier reported T_{fus} = 1188 K. $\Delta_{fus}H°$ = 28.8 kcal·mol^{-1} is from Smith.[3]

References

[1] L. Shartsis and W. Capps, J. Am. Ceram. Soc. 37, 27 (1954).
[2] U. S. Nat. Bur Stand. Circ. 500, 1268 pp. (1952).
[3] G. S. Smith, Ph. D. Thesis, Penn. State Univ., Univ Microfilms, Order No. Mic 59–2916 (1959).
[4] W. M. Latimer, J. Am. Chem. Soc. 73, 1480 (1951).
[5] K. K. Kelley, U. S. Bur. Mines, personal communication, (June, 1960).
[6] B. S. R. Sastry and F. A. Hummel, J. Am. Chem. Soc. 42, 216 (1959).
[7] A. P. Rollet and R. Bouaziz, Comp. Rend. 240. 2417 (1955).

Lithium Borate ($Li_2B_4O_7$) $B_4Li_2O_7$(cr)

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298 15	183.050	155.645	155 645	0.	−3362.262	−3170 291	555 422
300	183 096	156.777	155.648	0.339	−3362.289	−3169.100	551.789
400	197.648	211.259	162.980	19.311	−3364.367	−3104.421	405.396
500	219 940	257 778	177.378	40.200	−3372 974	−3038.519	317.432
600	241 103	299.795	194.332	63.278	−3374.846	−2971 434	258 686
700	259 199	338.357	212.190	88 317	−3375.669	−2904.120	216.708
800	274.412	373.983	230.216	115 013	−3375.575	−2836.753	185.221
900	287.717	407.078	248.050	143.125	−3374.692	−2769.445	160.734
1000	300.424	438.042	265.517	172.525	−3373.030	−2702.277	141.152
1100	314.018	467.306	282.543	203.239	−3370.479	−2635.316	125.141
1190.000	327.010	492.501	297.475	232.080	--- CRYSTAL <--> LIQUID ---		
1200	327.180	495.378	299.118	235.511	−3366.736	−2568.641	111.810
1300	340.343	522.086	315.249	268.887	−3362.211	−2502.310	100.544
1400	353.506	547.790	330.947	303.580	−3356 657	−2436.365	90.902
1500	366.669	572.628	346.236	339.589	−3350.045	−2370.856	82.561
1600	379.832	596.712	361.141	376.914	−3342.359	−2305.821	75.277
1700	392.995	620.135	375.690	415.555	−3624.059	−2226.948	68.426
1800	406 158	642.970	389.908	455.513	−3612.686	−2145.089	62.249
1900	419.320	665.283	403.816	496.786	−3600.229	−2063.890	56.740
2000	432.483	687.126	417.437	539.377	−3586.685	−1983.375	51.800

PREVIOUS: December 1962 CURRENT: June 1965

Lithium Borate ($Li_2B_4O_7$) $B_4Li_2O_7$(cr)

Lithium Borate ($Li_2B_4O_7$) LIQUID $M_r = 169.1178$ Lithium Borate ($Li_2B_4O_7$) $B_4Li_2O_7(l)$

$S°(298.15\ K) = [173.375]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298.15\ K) = [-3317.715]\ kJ{\cdot}mol^{-1}$

$T_{fus} = 1190 \pm 2\ K$ $\Delta_{fus}H° = 120.5 \pm 6.3\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

$\Delta_fH°(l,\ 298.15\ K)$ is calculated from $\Delta_fH°(cr,\ 298.15\ K)$ by adding the enthalpy of fusion and the difference in enthalpy, $H°(1190\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The enthalpy measurements of Smith[1] in the range 296 to 1373 K were smoothed graphically and used to determine C_p. The C_p data have a discontinuity at about 756 K. A linear extrapolation of C_p was used from 1373 to 3000 K.

The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Reference

[1] G. S. Smith, Ph. D. Thesis, Penn. State Univ., Univ. Microfilms, Order No. Mic. 59–2916 (1959).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200							
250							
298.15	181.146	173.375	173.375	0.	−3317.715	−3131.030	548.543
300	181.586	174.497	173.379	0.336	−3317.745	−3129.872	544.959
400	205.225	229.974	180.784	19.676	−3319.455	−3066.995	400.508
500	228.869	278.308	195.547	41.381	−3327.246	−3003.056	313.727
600	252.513	322.126	213.043	65.450	−3328.127	−2938.114	255.786
700	276.157	362.827	231.565	91.883	−3327.555	−2873.135	214.396
756.115	289.425	384.627	242.119	107.752	GLASS <--> LIQUID TRANSITION		
756.115	455.516	384.627	242.119	107.752			
800	456.746	410.361	250.649	127.769	−3318.272	−2808.552	183.380
900	459.549	464.319	271.448	173.584	−3299.686	−2745.956	159.371
1000	462.352	512.883	293.204	219.679	−3281.329	−2685.416	140.272
1100	465.156	557.081	315.213	266.055	−3263.117	−2626.707	124.732
1190.000	467.680	593.760	334.910	308.032	--- CRYSTAL <--> LIQUID ---		
1200	467.959	597.675	337.083	312.710	−3244.989	−2569.652	111.854
1300	470.762	635.243	358.592	359.646	−3226.905	−2514.108	101.018
1400	473.444	670.231	379.616	406.861	−3208.828	−2459.955	91.782
1500	475.836	702.977	400.094	454.325	−3190.762	−2407.096	83.823
1600	478.294	733.765	419.995	502.031	−3172.695	−2355.440	76.897
1700	480.818	762.836	439.315	549.986	−3445.081	−2290.563	70.380
1800	483.408	790.392	458.061	598.196	−3425.455	−2223.218	64.516
1900	486.063	816.600	476.247	646.669	−3405.799	−2156.962	59.299
2000	488.785	841.600	493.895	695.411	−3386.104	−2091.743	54.631
2100	491.572	865.515	511.026	744.429	−3366.359	−2027.510	50.432
2200	494.425	888.449	527.663	793.728	−3346.557	−1964.217	46.636
2300	497.344	910.491	543.832	843.316	−3326.690	−1901.830	43.192
2400	500.328	931.721	559.554	893.199	−3507.788	−1836.032	39.960
2500	503.379	952.207	574.853	943.384	−3488.083	−1766.780	36.915
2600	506.495	972.010	589.750	993.877	−3468.163	−1698.320	34.120
2700	509.677	991.185	604.264	1044.685	−3448.023	−1630.630	31.546
2800	512.925	1009.779	618.417	1095.814	−3427.657	−1563.690	29.171
2900	516.239	1027.837	632.225	1147.275	−3407.059	−1497.485	26.973
3000	519.297	1045.390	645.706	1199.054	−3386.242	−1431.991	24.933

PREVIOUS: December 1962 CURRENT: June 1965

Lithium Borate ($Li_2B_4O_7$) CRYSTAL-LIQUID

298.15 to 1190 K crystal
above 1190 K liquid

Refer to the individual tables for details.

M_r = 169.1178 Lithium Borate ($Li_2B_4O_7$) $B_4Li_2O_7(cr,l)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = p° = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	Δ_fH°	Δ_fG°	log K_f
0							
100							
200							
250							
298.15	183.050	155.645	155.645	0.	−3362.262	−3170.291	555.422
300	183.096	156.777	155.648	0.339	−3362.289	−3169.100	551.789
400	197.648	211.259	162.980	19.311	−3364.367	−3104.421	405.396
500	219.940	257.778	177.378	40.200	−3372.974	−3038.519	317.432
600	241.103	299.795	194.332	63.278	−3374.846	−2971.434	258.686
700	259.199	338.357	212.190	88.317	−3375.669	−2904.120	216.708
800	274.412	373.983	230.216	115.013	−3375.575	−2836.753	185.221
900	287.717	407.078	248.050	143.125	−3374.692	−2769.445	160.734
1000	300.424	438.042	265.517	172.525	−3373.030	−2702.277	141.152
1100	314.018	467.306	282.543	203.239	−3370.479	−2635.316	125.141
1190.000	327.010	492.501	297.475	232.080	CRYSTAL <−−> LIQUID TRANSITION		
1190.000	467.680	593.760	297.475	352.579			
1200	467.960	597.675	299.961	357.257	−3244.989	−2569.652	111.854
1300	470.762	635.243	324.324	404.194	−3226.905	−2514.108	101.018
1400	473.444	670.231	347.797	451.408	−3208.828	−2459.955	91.782
1500	475.836	702.977	370.396	498.872	−3190.762	−2407.096	83.823
1600	478.294	733.765	392.154	546.578	−3172.695	−2355.440	76.897
1700	480.818	762.836	413.111	594.533	−3445.081	−2290.563	70.380
1800	483.408	790.392	433.312	642.744	−3425.455	−2223.218	64.516
1900	486.063	816.600	452.801	691.217	−3405.799	−2156.962	59.299
2000	488.785	841.600	471.621	739.958	−3386.104	−2091.743	54.631
2100	491.572	865.515	489.813	788.976	−3366.359	−2027.510	50.432
2200	494.425	888.449	507.415	838.275	−3346.557	−1964.217	46.636
2300	497.344	910.491	524.464	887.863	−3326.690	−1901.830	43.192
2400	500.328	931.721	540.993	937.746	−3507.788	−1836.032	39.960
2500	503.379	952.207	557.034	987.931	−3488.083	−1766.780	36.915
2600	506.495	972.010	572.616	1038.424	−3468.163	−1698.320	34.120
2700	509.677	991.185	587.766	1089.232	−3448.023	−1630.630	31.546
2800	512.925	1009.779	602.507	1140.361	−3427.657	−1563.690	29.171
2900	516.239	1027.837	616.864	1191.822	−3407.059	−1497.485	26.973
3000	519.297	1045.390	630.857	1243.601	−3386.242	−1431.991	24.933

PREVIOUS: CURRENT: June 1965

Lithium Borate ($Li_2B_4O_7$) $B_4Li_2O_7(cr,l)$

Magnesium Boride (MgB_4) CRYSTAL $M_r = 67.545$ Magnesium Boride (MgB_4) $B_4Mg_1(cr)$

$S°(298.15\ K) = 51.92\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{dcm} = [1100]\ K$

$\Delta_f H°(0\ K) = -104.7 \pm 8.4\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -105.0 \pm 8.4\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The equilibrium pressures (1169–1177 K) of the reaction $MgB_4(cr) \rightarrow Mg(g) + 4B(cr)$ were measured by Wright and Walsh.[1] The 3rd law value of $\Delta_r H°(298.15\ K)$ for this reaction is derived as $60.40 \pm 1.5\ kcal{\cdot}mol^{-1}$. This leads to a $\Delta_f H°(298.15\ K) = -25.1 \pm 2.0\ kcal{\cdot}mol^{-1}$ for $MgB_4(cr)$. The unit of equilibrium pressures reported should be in atmosphere not in mm Hg as printed. The diameter of the hole drilled through the center of the lid served as the effusion orifice should be 1/16 inch rather than the reported value 1/6 inch.

Heat Capacity and Entropy

The low temperature (17.34–299.53 K) heat capacities were measured by Swift and White.[2] Above 298.15 K the C_p values are estimated by comparison with those of other related borides. $S°(298.15\ K)$ was reported by Swift and White[2] using $S°(\text{extrap., } 20\ K) = 0.022\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$.

Decomposition Data

T_{dcm} was estimated from the decomposition reaction reported by Wright and Walsh.[1]

References

[1] M. Wright and P. N. Walsh, Ohio State Univ. Research Foundation, 'Technical Research Report OMCC-HEF-55, (January 9, 1958).
[2] R. M. Swift and D. White, J. Am. Chem. Soc. 79, 3641 (1957).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.519	−104.683	−104.683	INFINITE
100	17.238	8.033	97.487	−8.945	−104.848	−104.578	54.626
200	46.275	28.702	57.635	−5.786	−105.028	−104.205	27.215
298.15	70.333	51.923	51.923	0.	−105.018	−103.801	18.185
300	70.710	52.360	51.925	0.130	−105.018	−103.793	18.072
400	79.496	73.935	54.807	7.651	−105.503	−103.339	13.495
500	87.027	92.491	60.529	15.981	−106.763	−102.664	10.725
600	94.140	109.006	67.256	25.050	−108.386	−101.695	8.853
700	99.956	123.955	74.305	34.755	−110.174	−100.440	7.495
800	105.730	137.684	81.380	45.043	−112.005	−98.924	6.459
900	111.043	150.450	88.354	55.887	−113.807	−97.180	5.640
1000	115.729	162.403	95.167	67.235	−124.164	−94.526	4.938
1100	118.512	173.561	101.793	78.945	−126.005	−91.473	4.344
1200	121.629	184.004	108.213	90.949	−127.787	−88.254	3.842
1300	125.525	193.897	114.427	103.311	−129.422	−84.892	3.411
1400	128.867	203.325	120.443	116.036	−258.297	−78.244	2.919
1500	131.587	212.311	126.270	129.062	−258.286	−65.382	2.277
1600	133.888	220.879	131.917	142.339	−258.193	−52.525	1.715
1700	135.562	229.046	137.393	155.811	−258.064	−39.674	1.219
1800	137.235	236.842	142.703	169.451	−257.921	−26.832	0.779
1900	138.909	244.307	147.855	183.258	−257.759	−13.998	0.385
2000	140.582	251.475	152.858	197.233	−257.573	−1.173	0.031

PREVIOUS: March 1963 CURRENT: March 1965

Sodium Borate ($Na_2B_4O_7$) **CRYSTAL** **M_r = 201.21534**

$S°(298.15\ K) = 189.49\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$T_{fus} = 1015.6\ K$

$\Delta_f H°(0\ K) = -3259.0 \pm 8\ kJ{\cdot}mol^{-1}$

$\Delta_f H°(298.15\ K) = -3276.7 \pm 8\ kJ{\cdot}mol^{-1}$

$\Delta_{fus} H° = 76\ 9 \pm 6.3\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The enthalpy of the reaction $Na_2O(cr) + 2B_2O_3(l) \rightarrow Na_2B_4O_7(cr)$ was reported by Shartsis and Capps[1] from their enthalpy of solution measurements Their values for the enthalpy of reaction of the oxides have been converted to the enthalpy of formation using JANAF values[2] for $B_2O_3(l)$ and for $Na_2O(cr)$. The above $\Delta_f H° = -85.2\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

In the low temperature region (5–344 K) the C_p values are those determined by Westrum and Grenier.[3] The enthalpy measurements of Smith[4] in the range 296 to 1015.6 K were smoothed graphically and used to determine C_p, the values did not join smoothly with those of Westrum and Grenier and the low temperature values were given greater weight. Above T_{fus} the heat capacity was extrapolated. $S°(298.15\ K)$ was derived from low temperature heat capacities.

Fusion Data

The value for T_{fus} is from Morey and Merwin.[5] Other reported values are 1008 ± 5 K by Coles, Scholes, and Amberg;[6] 1011 K by Menzel;[7] 1005 K by Ponomareff;[8] 1015 K by Day and Allen;[9] and 1064 K by Burgess and Holt.[10] $\Delta_{fus}H°$ was obtained from the values of $\Delta_f H°$ for $Na_2B_4O_7(cr)$ and $Na_2B_4O_7(l)$ at 298.15 K as described above and the difference between $H°(1015\ K)–H°(298.15\ K)$ for crystal and liquid.

References

[1] L. Shartsis and W. Capps, J. Am. Ceram. Soc. 37, 27 (1954).
[2] JANAF Thermochemical Tables: $B_2O_3(l)$, 12–31–64; $Na_2O(cr)$, 6–30–62.
[3] E. F. Westrum, Jr. and G. Grenier, J. Am. Chem. Soc. 79, 1799 (1957).
[4] G. S. Smith, Ph. D. Thesis, Penn. Stae Univ., Univ. Microfilms, Order No. Mic 59–2916 (1959).
[5] G. W. Morey and H. E. Merwin, J. Am. Chem. Soc. 58, 2248 (1936).
[6] S. S. Coles, S. R. Scholes, and C. R. Amberg, J. Am. Ceram. Soc. 18, 58 (1935).
[7] H. Menzel, Z. anorg. Chem. 224, 1 (1935).
[8] J. F. Ponomareff, Z. anorg. Chem. 89, 383 (1924).
[9] A. L. Day and E. T. Allen, Carnegie Inst. of Washington, Publ. No. 31, 29 (1905).
[10] C. H. Burgess and Q. Holt, Proc. Roy. Soc. (London) 74, 285 (1904).

Sodium Borate ($Na_2B_4O_7$) **$B_4Na_2O_7(cr)$**

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0	INFINITE	−30.382	−3258.983	−3258.983	INFINITE
100	76.525	50 814	321.976	−27.116	−3268.658	−3208.196	1675.790
200	139 746	124.566	205.130	−16.113	−3274.087	−3145.347	821.480
298.15	186.774	189 490	189.490	0.	−3276.741	−3081.522	539.870
300	187 447	190.648	189 494	0.346	−3276.774	−3080.310	536.330
400	213 802	248.460	197 196	20.505	−3283.707	−3014.160	393.609
500	228.534	297.784	212.510	42.637	−3285.408	−2946.574	307.826
600	241.500	340.624	230.368	66.154	−3286.907	−2878.661	250.610
700	252.697	378.715	248.889	90.878	−3288.098	−2810.522	209.724
800	262.128	413.077	267.299	116.622	−3288.983	−2742.233	179.049
900	271.215	444.482	285.266	143.294	−3289.531	−2673.853	155.186
1000	279.700	473.502	302.657	170.845	−3289.721	−2605.430	136.094
1015.600	280.970	477.841	305.314	175.218	--- CRYSTAL <--> LIQUID ---		
1100	287.583	500.534	319.431	199.214	−3289.570	−2537.005	120.472
1200	294.863	525.874	335.589	228.342	−3482.640	−2463.728	107.243
1300	301.541	549.743	351.153	258.167	−3480.079	−2378.921	95.586
1400	307.616	572.316	366.152	288.630	−3477.180	−2294.323	85.602
1500	313.089	593.718	380.616	319.653	−3473.995	−2209.943	76.957
1600	320.013	614.144	394.577	351.307	−3470.439	−2125.786	69.400
1700	327.017	633.755	408.074	383.658	−3466.432	−2041.866	62.739
1800	334.105	652.647	421.139	416.714	−3461.958	−1958.196	56.825
1900	341.276	670.903	433.807	450.482	−3457.003	−1874.786	51.541
2000	348.527	688.592	446.106	484.972	−3451.552	−1791.650	46.793

PREVIOUS: March 1963 CURRENT: March 1965

Sodium Borate ($Na_2B_4O_7$) **$B_4Na_2O_7(cr)$**

$S°(298.15\ K) = [194.636]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 1015.6\ K$

$\Delta_fH°(298.15\ K) = [-3256.658]\ kJ{\cdot}mol^{-1}$
$\Delta_{fus}H° = 76.9 \pm 6.3\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The enthalpy of reaction $Na_2O(cr) + 2B_2O_3(l) \rightarrow Na_2B_4O_7(l)$ was reported by Shartsis and Capps[1] from their enthalpy of solution measurements. Their values for the enthalpy of reaction of the oxides have been converted to the enthalpies of formation using JANAF values[2] for $B_2O_3(l)$ and $Na_2O(cr)$. The above $\Delta_rH° = -80.4\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

The enthalpy measurements of Smith[3] in the range 298 to 1373 K, were smoothed graphically and used to determine C_p. These were joined smoothly with the low temperature data of Westrum and Grenier.[4] At 743 K a glass transition was observed and above this temperature the C_p adopted as constant.

The entropy at 298.15 K is calculated from that of the crystal by adding $\Delta_{fus}S°$ and the difference in entropy, $S°(1015\ K)-S°(298.15\ K)$, between the crystal and liquid.

Fusion Data

Refer to the crystal table for details.

References

[1] L. Shartsis and W. Capps, J. Am. Ceram. Soc. 37, 27 (1954).
[2] JANAF Thermochemical Tables: $B_2O_3(l)$, 12–31–64; $Na_2O(cr)$, 6–30–62.
[3] G. S. Smith, Ph. D. Thesis, Penn. State Univ., Univ. Microfilms, Order No. Mic 59–2916 (1959).
[4] E. F. Westrum, Jr. and G. Grenier, J. Am. Chem. Soc. 79, 1799 (1957).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	$\log K_f$
0							
100							
200							
298.15	187.443	194.636	194.636	0.	−3256.658	−3062.973	536.620
300	188.141	195.798	194 640	0.347	−3256.690	−3061.771	533.102
400	221.752	254.719	202.445	20.909	−3263.220	−2996.176	391.260
500	247.274	307.021	218.230	44.396	−3263.566	−2929.350	306.027
600	268.613	353.997	237.008	70.194	−3262.784	−2862.562	249.208
700	289.533	396.980	256.831	98.104	−3260.789	−2795.998	208.640
743.010	298.402	414.507	265.454	110.748	GLASS <--> LIQUID		
743.010	444.885	414.507	265.454	110.748	TRANSITION		
800	444.885	447.385	277.257	136.102	−3249.420	−2730.116	178.258
900	444.885	499.785	299.129	180.591	−3232.152	−2666.246	154.745
1000	444.885	546.658	321.579	225.079	−3215.404	−2604.270	136.033
1015.600	444.885	553.544	325.089	232.019	--- CRYSTAL <--> LIQUID ---		
1100	444.885	589.060	343.999	269.567	−3199.134	−2543.947	121.802
1200	444.885	627.770	366.057	314.056	−3376.842	−2480.207	107.961
1300	444.885	663.380	387.577	358.544	−3359.618	−2406.188	96.682
1400	444.885	696.350	408.469	403.033	−3342.693	−2333.483	87.063
1500	444.885	727.043	428.696	447.521	−3326.043	−2261.980	78.769
1600	444.885	755.756	448.249	492.010	−3309.653	−2191.579	71.548
1700	444.885	782.727	467.139	536.498	−3293.508	−2122.194	65.207
1800	444.885	808.156	485.385	580.987	−3277.602	−2053.755	59.598
1900	444.885	832.209	503.012	625.475	−3261.926	−1986.192	54.604
2000	444.885	855.029	520.047	669.964	−3246.476	−1919.448	50.131
2100	444.885	876.735	536.519	714.452	−3231.250	−1853.472	46.103
2200	444.885	897.431	552.458	758.941	−3216.243	−1788.214	42.458
2300	444.885	917.207	567.890	803.429	−3201.454	−1723.637	39.145
2400	444.885	936.141	582.842	847.918	−3387.918	−1655.423	36.029
2500	444.885	954.302	597.340	892.406	−3373.872	−1583.525	33.086
2600	444.885	971.751	611.407	936.895	−3359.910	−1512.187	30.380
2700	444.885	988.541	625.066	981.383	−3346.033	−1441.383	27.885
2800	444.885	1004.720	638.337	1025.872	−3332.239	−1371.092	25.578
2900	444.885	1020.332	651.242	1070.360	−3318.532	−1301.296	23.439
3000	444.885	1035.414	663.798	1114.848	−3304.911	−1231.967	21.450

PREVIOUS: March 1963 CURRENT: March 1965

Sodium Borate ($Na_2B_4O_7$) CRYSTAL-LIQUID

0	to 1015.6 K	crystal
above	1015.6 K	liquid

Refer to the individual tables for details.

M_r = 201.21534 Sodium Borate ($Na_2B_4O_7$) $B_4Na_2O_7$(cr,l)

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−30.382	−3258.983	−3258.983	INFINITE
100	76.525	50.814	321.976	−27.116	−3268.658	−3208.196	1675.790
200	139.746	124.566	205.130	−16.113	−3274.087	−3145.347	821.480
298.15	186.774	189.490	189.490	0.	−3276.741	−3081.522	539.870
300	187.447	190.648	189.494	0.346	−3276.774	−3080.310	536.330
400	213.802	248.460	197.196	20.505	−3283.707	−3014.160	393.609
500	228.534	297.784	212.510	42.637	−3285.408	−2946.574	307.826
600	241.500	340.624	230.368	66.154	−3286.907	−2878.661	250.610
700	252.697	378.715	248.889	90.878	−3288.098	−2810.522	209.724
800	262.128	413.077	267.299	116.622	−3288.983	−2742.233	179.049
900	271.215	444.482	285.266	143.294	−3289.531	−2673.853	155.186
1000	279.700	473.502	302.657	170.845	−3289.721	−2605.430	136.094
1015.600	280.970	477.841	305.314	175.218	CRYSTAL <--> LIQUID TRANSITION		
1015.600	444.885	553.544	305.314	252.102			
1100	444.885	589.060	325.741	289.651	−3199.134	−2543.946	120.802
1200	444.885	627.770	349.320	334.139	−3376.842	−2480.206	107.961
1300	444.885	663.379	372.127	378.628	−3359.618	−2406.187	96.682
1400	444.893	696.349	394.123	423.117	−3342.693	−2333.483	87.063
1500	444.885	727.043	415.306	467.605	−3326.043	−2261.980	78.769
1600	444.885	755.756	435.697	512.094	−3309.652	−2191.578	71.548
1700	444.885	782.727	455.325	556.582	−3293.507	−2122.194	65.207
1800	444.885	808.156	474.227	601.071	−3277.601	−2053.754	59.598
1900	444.885	832.209	492.441	645.559	−3261.925	−1986.191	54.604
2000	444.885	855.029	510.005	690.048	−3246.476	−1919.447	50.131
2100	444.885	876.735	526.956	734.536	−3231.249	−1853.471	46.103
2200	444.885	897.431	543.329	779.025	−3216.242	−1788.213	42.458
2300	444.885	917.207	559.158	823.513	−3201.453	−1723.636	39.145
2400	444.885	936.141	574.473	868.002	−3387.917	−1655.422	36.029
2500	444.885	954.302	589.306	912.490	−3373.871	−1583.524	33.086
2600	444.885	971.751	603.682	956.979	−3359.909	−1512.186	30.380
2700	444.885	988.541	617.627	1001.467	−3346.032	−1441.382	27.885
2800	444.885	1004.720	631.165	1045.956	−3332.239	−1371.091	25.578
2900	444.885	1020.332	644.317	1090.444	−3318.531	−1301.295	23.439
3000	444.885	1035.414	657.103	1134.933	−3304.910	−1231.967	21.450

PREVIOUS: CURRENT: March 1965

Sodium Borate ($B_2Na_4O_7$) $B_4Na_2O_7$(cr,l)

Lead Borate (PbB_4O_7) CRYSTAL $M_r = 362.4358$ Lead Borate (PbB_4O_7) $B_4O_7Pb_1(cr)$

$\Delta_fH°(0\ K)$ = Unknown

$S°(298.15\ K) = [166.9 \pm 13]\ J·K^{-1}·mol^{-1}$ (298.15 K) = $[-2858 \pm 6]\ kJ·mol^{-1}$

Enthalpy of Formation

See the $PbB_2O_4(cr)$ table for the complete writeup. Evans[1] analysed the enthalpies of formation of lead borate system based upon Shartsis and Newman's enthalpies of solution and Mazzetti and DeCarli's phase studies. From the Shartsis and Newman paper Evans obtained the following:

$$PbO(cr) + 2B_2O_3(cr) \rightarrow PbO·2B_2O_3(gl) \qquad \Delta_rH = -11.9\ kcal·mol^{-1}$$

and estimated a $\Delta_fH°(298.15\ K)$ value of 11.4 $kcal·mol^{-1}$ for the conversion to the $PbO·2B_2O_3(cr)$. With auxiliary JANAF values $\Delta_fH°(298.15\ K)$ is calculated to be $-683.00\ kcal·mol^{-1}$.

Heat Capacity and Entropy

The heat capacity employed in this table is obtained by graphically smoothing the summation of the heat capacities of the constituent oxides.

The entropy at 298.15 K is obtained from a consideration of the entropies of sodium and calcium borates and those of the constituent oxides, as given by Kelley and King.[2] These indicate for the reaction:

$$MO·B_2O_3 + B_2O_3 \rightarrow MO·2B_2O_3$$

that the simple addition of entropies will give values at least 2.7 $cal·K^{-1}·mol^{-1}$ in case of Na borates and 5.7 $cal·K^{-1}·mol^{-1}$ for Ca borates too high for the reaction. The reason for this is probably structural, the $B_4O_7^{=}$ ion is a rigid chain of rings. It was assumed that additional B_2O_3 would extend the ring structure into a rigid plane and thus the average entropy difference of 4.2 for the reaction was assumed to hold for each additional mole of B_2O_3. Therefore the entropy at 298.15 K is obtained from $S°(298.15\ K)$ for PbB_2O_4 and B_2O_3 and the subtraction of 4.2 $cal·K^{-1}·mol^{-1}$.

References

[1] W. H. Evans, U. S. Nat. Bur. Stand. Report 7192, Ch. 6 (July 1, 1961); refer to pp. 80–1.

[2] K. K. Kelly and E. G. King, U. S. Bur. Mines, Bull. 592, 149 pp. (1961).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200							
250							
298.15	168.197	166.942	166.942	0.	−2857.672	−2667.096	467.264
300	169.034	167.985	166.945	0.312	−2857.684	−2665.914	464.177
400	206.522	221.877	174.039	19.135	−2857.439	−2601.980	339.784
500	238.572	271.498	188.634	41.432	−2855.586	−2538.298	265.174
600	265.558	317.462	206.323	66.683	−2852.207	−2475.133	215.480
700	287.148	360.073	225.282	94.354	−2852.370	−2411.845	179.974
800	304.512	399.590	244.632	123.967	−2846.584	−2349.295	153.393
900	318.277	436.271	263.912	155.123	−2839.860	−2287.529	132.765
1000	330.034	470.433	282.876	187.558	−2832.345	−2226.555	116.303
1100	339.490	502.348	301.393	221.050	−2824.179	−2166.366	102.872
1200	347.021	532.225	319.398	255.393	−2815.507	−2106.944	91.713
1300	352.502	560.226	336.858	290.378	−2806.499	−2048.261	82.300
1400	356.853	586.512	353.761	325.851	−2797.295	−1990.279	74.258
1500	360.577	611.264	370.111	361.730	−2787.962	−1932.961	67.312
1600	363.422	634.629	385.920	397.935	−2778.570	−1876.267	61.254
1700	365.682	656.732	401.206	434.395	−2769.182	−1820.160	55.927
1800	367.397	677.685	415.989	471.052	−2759.850	−1764.606	51.208
1900	368.694	697.585	430.290	507.859	−2750.617	−1709.567	46.999
2000	369.740	716.524	444.132	544.782	−2741.512	−1655.011	43.224

PREVIOUS: December 1962 CURRENT: March 1965

Pentaborane (B_5H_9) LIQUID $M_r = 63.12146$ Pentaborane (B_5H_9) $B_5H_9(l)$

$S°(298.15\ K) = 184.33\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298.15\ K) = 42.84 \pm 6.7\ kJ{\cdot}mol^{-1}$

$T_{fus} = 226.34\ K$ $\Delta_{fus}H° = 6.134\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The vapor pressures of $B_5H_9(l)$ were measured by Wirth and Palmer[1] and Johnston, Kerr, Clarke and Hallett.[2] By use of both the 2nd and 3rd law methods, the respective enthalpies of vaporization are evaluated. The $\Delta_fH°(298.15\ K)$ values for $B_5H_9(l)$ are calculated from $\Delta_fH°(298.15\ K)$ for $B_5H_9(g)$ and $\Delta_{vap}H°(298.15\ K)$ for $B_5H_9(l)$ obtained previously.

Source	$\Delta_rH°(298.15\ K)$, kcal·mol⁻¹ 2nd law	3rd law	$\Delta_fH°(298.15\ K)$ kcal·mol⁻¹
Wirth and Palmer[1]	7.26 ± 0.02	7.26	10.24 ± 1.6
Johnston, *et al.*[2]	7.23 ± 0.04	7.25	10.23 ± 1.6

The adopted value is the average of the two $\Delta_fH°(298.15\ K)$ values obtained.

Heat Capacity and Entropy

The heat capacities, 231.34–290.19 K, for $B_5H_9(l)$ were measured by Johnston, Kerr, Clarke and Hallett.[2] The C_p values above 290.19 K are estimated by graphical extrapolation of the C_p curve plotted using the experimental data. The value of $S°(298.15\ K)$ was derived based on the low temperature C_p, 13.29–221.61 K, and $\Delta_{fus}H°$ for $B_5H_9(cr)$ reported by Johnston, Kerr, Clarke and Hallett[2] and C_p values, 226.34–298.15 K, for $B_5H_9(l)$, using $S°(13.29\ K) = 0.236\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ for $B_5H_9(cr)$.

Fusion Data

The values of T_{fus} and $\Delta_{fus}H°$ were taken from Johnston, Kerr, Clarke and Hallett.[2]

Vaporization Data

The boiling point is calculated as the temperature at which the Gibbs energy change of the reaction $B_5H_9(l) \rightarrow B_5H_9(g)$ is zero. The enthalpy change of the reaction at T_{vap} is enthalpy of vaporization.

References

[1] H. E. Wirth and E. D. Palmer, J. Phys. Chem. 60, 914 (1956).
[2] H. L. Johnston, E. c. Kerr, J. T. Clarke, and N. Cl Hallet, The Ohio State University, TR-6, (July 8, 1949).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_fH°$ (kJ·mol⁻¹)	$\Delta_fG°$ (kJ·mol⁻¹)	log K_f
0							
100							
200							
298.15	151.126	184.330	184.330	0.	42.844	171.913	−30.118
300	152.298	185.269	184.333	0.281	42.780	172.714	−30.072
400	185.351	233.939	190.744	17.278	39.888	216.489	−28.271
500	190.372	275.566	203.682	35.942	36.745	260.981	−27.264
600	210.037	311.791	218.723	55.841	33.557	306.142	−26.652
700	244.346	347.030	234.537	78.745	32.465	351.697	−26.244
800	256.479	380.470	250.719	103.801	32.820	397.284	−25.940
900	267.096	411.315	266.871	130.000	33.724	442.793	−25.699
1000	275.307	439.903	282.763	157.140	35.036	488.177	−25.500
1100	280.272	466.381	298.267	184.925	36.497	533.421	−25.330
1200	284.512	490.955	313.313	213.170	37.945	578.532	−25.183
1300	288.027	513.872	327.869	241.803	39.327	623.524	−25.054
1400	290.816	535.323	341.929	270.751	40.588	668.414	−24.939
1500	292.880	555.462	355.500	299.942	41.671	713.219	−24.837

PREVIOUS: December 1962 CURRENT: March 1965

Pentaborane (B_5H_9) IDEAL GAS $M_r = 63.12146$ Pentaborane (B_5H_9) B_5H_9(g)

$S°(298.15\ K) = 275.41\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 102.23 \pm 6.7\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 73.22 \pm 6.7\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies

υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}	υ, cm^{-1}
2600 (1)	[1450](1)	[1500](1)	1449 (2)
2600 (1)	[500](1)	[1100](1)	1034 (2)
1844 (1)	1870 (1)	738 (1)	882 (2)
1413 (1)	1387 (1)	470 (1)	700 (2)
1126 (1)	[900] (1)	2598 (2)	605 (2)
985 (1)	782 (1)	1802 (2)	568 (2)
799 (1)	2600 (1)	1621 (2)	

Ground State Quantum Weight: 1 $\sigma = 4$
Point Group: C_{4v}
Bond Distances: B–B = 1.800 ± 0.003 Å; B–B(apex) = 1.687 ± 0.005 Å
B–H = B(apex)–H = 1.22 Å; B–H(bridge) = 1.35 ± 0.02 Å
Bond Angles: B(apex)–B–H = 136° 10' ± 30'; H–B(apex)–B = 131°:
B–H(bridge)–B = 83° 37'; B–B–B = 90°
Angle between B(apex)BB plane and BBH(bridge) plane = 196 ± 2°
Product of the Moments of Inertia: $I_AI_BI_C = 2.366493 \times 10^{-114}\ g^3\ cm^6$

Enthalpy of Formation

The enthalpy change[2] of the reaction $B_5H_9(g) \rightarrow 5\ B(am) + 9/2\ H_2(g)$ was reported to be −12.99 ± 0.39 and −9.9 ± 1 $kcal{\cdot}mol^{-1}$ by Prosen, Johnson and Pergiel[1] and Gunn and Green,[2] respectively. Using $\Delta_rH°(298\ 15\ K) = 1.2 \pm 0.4\ kcal{\cdot}mol^{-1}$ for the reaction $B(cr) \rightarrow B(am)$, the corresponding $\Delta_fH°(298.15\ K)$ values for $B_5H_9(g)$ were derived as 18.99 and 15.9 $kcal{\cdot}mol^{-1}$. The adopted value is the average of these two.

Heat Capacity and Entropy

The molecular structure, a tetragonal pyramid of boron atoms, and constants were obtained from Hrostowski and Myers.[3] The vibrational frequencies were reported by Hrostowski and Pimentel.[4] The earlier models of pentaborane were assumed to have a hydrocarbon-like structure of low symmetry by Bauer and Pauling,[5] and Pitzer.[6] However, the electron diffraction and X-ray data by Hedberg, Jones and Schomaker,[7] and Dulmage and Lipscomb[8] revealed an unusual pyramidal structure of C_{4v} symmetry. The Raman spectrum of liquid B_5H_9 and the infrared spectrum of gaseous B_5H_9 from 3 to 25 microns have been obtained by Taylor, Beckett, Tung, Holden and Johnston.[9] The near infrared spectrum of $B_5H_9(l)$ have been examined at high resolution by Pondy and Beachell.[10] Ten bands were observed. The principal moments of inertia are: $I_A = 16.9101 \times 10^{-39}$, and $I_B = I_C = 11\ 8299 \times 10^{-39}\ g\ cm^2$.

References

[1] E. J Prosen, W. H. Johnson, and F. Y. Pergiel, J. Res. Nat. Bur. Stand. 61, 247 (1958).
[2] S. R. Gunn and L. G. Green, J. Phys. Chem. 65, 2173 (1961).
[3] H. J Hrostowski and R. J. Myers, J. Chem. Phys. 22, 262 (1954).
[4] H. J. Hrostowski and G. C. Pimental, J. Am. Chem. Soc. 76, 998 (1954).
[5] S. H. Bauer and L. Pauling, J Am. Chem. Soc. 58, 2403 (1936).
[6] K. S Pitzer, J. Am. Chem. Soc. 67, 1126 (1945).
[7] K. Hedberg, M. E. Jones, and V Schomaker, Proc. Natl. Acad. Sci., U S 38, 679 (1952).
[8] W. J Dulmage and W N. Liscomb, Acta Cryst 5, 260 (1952).
[9] W. C. Taylor, C. W. Beckett, J. Y Tung, R. B Holden, and H L Johnston, Phys. Rev. 79, 234 (1950).
[10] P R. Pondy and H C. Beachill, J. Chem. Phys 25, 238 (1956).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	S°	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−15.163	102.230	102.230	INFINITE
100	34.678	216.114	334.297	−11.818	91.958	115.828	−60.502
200	57.782	245.727	282.800	−7.415	82.575	143.319	−37.431
250	75.771	260.522	276.853	−4.083	77.768	159.061	−33.234
298.15	93.818	275.410	275.410	0.	73.220	175.133	−30.683
300	94.509	275.993	275.412	0.174	73.049	175.766	−30.604
350	112.830	291.947	276.630	5.361	68.579	193.243	−28.840
400	130.205	308.160	279.557	11.441	64.427	211.339	−27.598
450	146.409	324.443	283.639	18.362	60.637	229.935	−26.690
500	161.367	340.654	288.531	26.061	57.240	248.932	−26.006
600	187.614	372.467	299.884	43.550	51.642	287.822	−25.057
700	209.395	403.077	312.455	63.435	47.531	327.530	−24.441
800	227.365	432.249	325.622	85.302	44.697	367.737	−24.011
900	242.175	459.912	339.020	108.803	42.903	408.234	−23.693
1000	254 403	486.081	352.430	133.651	41.923	448.886	−23.447
1100	264.538	510.819	365.715	159.614	41.561	489.604	−23.249
1200	272.980	534.209	378.791	186.502	41.653	530.334	−23.085
1300	280.052	556.347	391.605	214.164	42.064	571.043	−22.945
1400	286.013	577.325	404.128	242.476	42.688	611.711	−22.823
1500	291.069	597.235	416.344	271.337	43.441	652.330	−22.716
1600	295.384	616.162	428.246	300.665	44.258	692.895	−22.621
1700	299.088	634.183	439.834	330.393	45.084	733.410	−22.535
1800	302.287	651.371	451.113	360.466	45.882	773.877	−22.457
1900	305.064	667.791	462.088	390.836	46.617	814.300	−22.387
2000	307.488	683.502	472.769	421.467	47.264	854.688	−22.322
2100	309.615	698.557	483.165	452.324	47.805	895.045	−22.263
2200	311.489	713.005	493.286	483.381	48.222	935.379	−22.209
2300	313.149	726.888	503.143	514.615	48.503	975.698	−22.159
2400	314.625	740.247	512.745	546.005	−202.660	1021.352	−22.229
2500	315.942	753.118	522.104	577.535	−203.071	1072.361	−22.406
2600	317.122	765.533	531.230	609.189	−203.482	1123.386	−22.569
2700	318.183	777.522	540.131	640.955	−203.899	1174.427	−22.721
2800	319.141	789.111	548.817	672.822	−204.330	1225.484	−22.862
2900	320.007	800.325	557.298	704.780	−204.779	1276.557	−22.993
3000	320.793	811.187	565.581	736.821	−205.251	1327.645	−23 116
3100	321.509	821.718	573.674	768.936	−205.750	1378.749	−23.232
3200	322.163	831.936	581.586	801.121	−206.279	1429.871	−23.340
3300	322.761	841.859	589.323	833.367	−206.843	1481.010	−23.442
3400	323.309	851.502	596.893	865.671	−207.444	1532.165	−23.539
3500	323.814	860.882	604.302	898.028	−208.084	1583.339	−23.630
3600	324.278	870.010	611.557	930.432	−208.766	1634.532	−23.716
3700	324.707	878.901	618.663	962.882	−209.493	1685.745	−23 798
3800	325.104	887.566	625.626	995.373	−210.265	1736.978	−23.876
3900	325.472	896.016	632.451	1027.902	−211.086	1788.232	−23.951
4000	325.814	904.260	639.144	1060.466	−211.957	1839.507	−24.021
4100	326.131	912.309	645.708	1093.064	−212.878	1890.806	−24.089
4200	326.427	920.172	652.150	1125.692	−2613.099	1977.248	−24.591
4300	326.704	927.856	658.473	1158.349	−2608.690	2086.489	−25.346
4400	326.962	935.370	664.681	1191.032	−2604.344	2195.629	−26.065
4500	327.203	942.720	670.778	1223.740	−2600.062	2304.670	−26.752
4600	327.430	949.914	676.768	1256.472	−2595.847	2413.618	−27.407
4700	327.642	956.959	682.655	1289.226	−2591.698	2522.474	−28.034
4800	327.842	963.859	688.442	1322.000	−2587.617	2631.245	−28 634
4900	328.030	970.620	694.132	1354.794	−2583.605	2739 928	−29.208
5000	328.207	977.249	699.728	1387.606	−2579.661	2848.533	−29.758
5100	328.374	983.750	705.234	1420.435	−2575.787	2957.056	−30.286
5200	328.531	990.128	710.651	1453.280	−2571.983	3065.507	−30.793
5300	328.680	996.388	715.984	1486.141	−2568.247	3173.885	−31.281
5400	328.821	1002.533	721.233	1519 016	−2564.579	3282 193	−31 749
5500	328.955	1008.568	726.403	1551 905	−2560 978	3390 432	−32.200
5600	329.081	1014 496	731.495	1584.807	−2557.444	3498.608	−32.634
5700	329 201	1020.322	736.511	1617.721	−2553 975	3606.721	−33 052
5800	329.315	1026.048	741 454	1650.647	−2550.569	3714 775	−33 455
5900	329 423	1031 678	746.325	1683.584	−2547.226	3822.767	−33 844
6000	329 526	1037.216	751.127	1716.531	−2543 942	3930.705	−34.220

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

Potassium Borate ($K_2B_6O_{10}$) CRYSTAL $M_r = 303.0506$ Potassium Borate ($K_2B_6O_{10}$) $B_6K_2O_{10}(cr)$

$S°(298.15 K) = [251 \pm 13]$ J·K⁻¹·mol⁻¹ $\Delta_fH°(0 K)$ = Unknown

T_{dcm} = 1098 K $\Delta_fH°(298.15 K) = -4633.53 \pm 10.4$ kJ·mol⁻¹

Enthalpy of Formation

The enthalpy of reaction $K_2O(cr) + 3B_2O_3(l) \rightarrow K_2B_6O_{10}(cr)$ was reported by Shartsis and Capps[1] from their enthalpy of solution measurements. Their values for the enthalpy of reaction of the oxides have been converted to the enthalpies of formation using JANAF values[2] for $B_2O_3(l)$ and for $K_2O(cr)$. The above $\Delta_fH° = -122.8$ kcal·mol⁻¹.

Heat Capacity and Entropy

The enthalpy measurements of Smith[3] in the range 298 to 973 K were graphically smoothed and used to determine C_p. Above this range C_p is extrapolated.

The entropy at 298.15 K is obtained from a consideration of the entropies of sodium and calcium borates and those of the constituent oxides, as given by Kelley and King.[4] These indicate that for the reactions

$$MO + B_2O_3 \rightarrow MO{\cdot}B_2O_3 \qquad (1)$$

$$MO{\cdot}B_2O_3 + B_2O_3 \rightarrow MO{\cdot}2B_2O_3 \qquad (2)$$

the simple addition of entropies will give values at least 2.7 cal·K⁻¹mol⁻¹ too low for the reaction[1] and at least 2.7 cal·K⁻¹mol⁻¹ too high for reaction[2]. The reason for this is probably structural, the $B_2O_4^-$ ion being a flexible chain while the $B_4O_7^=$ on probably is a rigid chain of rings. It was assumed that additional B_2O_3 would extend the ring structure into a rigid plane and thus the entropy difference for reaction[2] was assumed to hold for each additional mole of B_2O_3 added. Thus a value for $Na_2B_6O_{10}$ was estimated to be 55.5 ± 1.5 and then using an average value of 4.5 ± 1.5 cal·K⁻¹mol⁻¹ for the difference between K_2 and Na_2 gave 60 ± 3 cal·K⁻¹·mol⁻¹ for the entropy fo $K_2B_6O_{10}$.

Decomposition Data

The incongruent melting point was given by Rollet[5] the decomposition products being $K_2B_4O_7(l)$ and $K_2B_8O_{13}(cr)$.

References

[1] L. Shartsis and W. Capps, J. Am. Ceram. Soc. 37, 27 (1954).

[2] JANAF Thermochemical Tables: $B_2O_3(l)$, 12–31–64; $K_2O(cr)$, 6–30–63.

[3] G. S. Smith, Ph.D. Thesis, Penn. State Univ., Univ. Microfilms, Order No. Mic 59–2916 (1959).

[4] K. K. Kelley and E. G. King, U.S. Bur. Mines, Bull. 592, 149 pp. (1961).

[5] A.-P. Rollet, Comp. rend. 200, 1763 (1935).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200							
250							
298.15	261.918	251.040	251.040	0.	−4633.529	−4353.554	762.725
300	262.337	252.661	251.045	0.485	−4633.551	−4351.817	757.719
400	285.767	331.362	261.617	27.898	−4640.126	−4256.761	555.876
500	308.277	397.560	282.348	57.606	−4642.314	−4160.664	434.662
600	330.118	455.703	306.487	89.530	−4644.154	−4064.153	353.816
700	351.456	508.194	331.610	123.608	−4645.271	−3967.385	296.050
800	372.794	556.524	356.742	159.826	−4645.388	−3870.524	252.719
900	393.463	601.639	381.473	198.150	−4644.347	−3773.716	219.021
1000	412.835	644.176	405.636	238.539	−4642.067	−3677.091	192.072
1100	423.295	684.043	429.155	280.376	−4796.992	−3571.514	169.597
1200	430.073	721.173	451.961	323.055	−4791.748	−3460.337	150.625
1300	435.680	755.823	474.018	366.347	−4786.378	−3349.604	134.589
1400	440.659	788.294	495.318	410.167	−4780.923	−3239.287	120.859
1500	445.387	818.859	515.879	454.471	−4775.390	−3129.364	108.974
1600	449.864	847.747	535.726	499.234	−4769.782	−3019.811	98.587
1700	454.299	875.154	554.893	544.443	−4764.094	−2910.611	89.432
1800	458.622	901.244	573.416	590.090	−4758.324	−2801.750	81.305
1900	462.834	926.153	591.330	636.164	−4752.475	−2693.210	74.042
2000	466.934	949.998	608.672	682.653	−4746.552	−2584.980	67.513

PREVIOUS: March 1963 CURRENT: March 1965

Lithium Borate ($Li_2B_6O_{10}$) CRYSTAL M_r = 238.7360 Lithium Borate ($Li_2B_6O_{10}$) $B_6Li_2O_{10}$(cr)

$\Delta_f H°$(0 K) = Unknown

$S°$(298.15 K) = [188.3 ± 4] J·K^{-1}·mol^{-1} $\Delta_f H°$(298.15 K) = −4659.89 ± 5.6 kJ·mol^{-1}

T_{dcm} = 1107 ± 4 K

Enthalpy of Formation

The enthalpy of reaction $Li_2O(cr) + 3B_2O_3(l) \rightarrow Li_2B_6O_{10}(cr)$ was reported by Shartsis and Capps[1] from their enthalpy of solution measurements. Their values for the enthalpy of reaction of the oxides have been converted to the enthalpies of formation using JANAF values[2] for B_2O_3(l) and Li_2O(cr). The above $\Delta_r H°$ = −72.80 kcal·mol^{-1}.

Heat Capacity and Entropy

The enthalpy measurement of Smith[3] in the range 298 to 823 K were used to determine C_p. Above this range C_p is extrapolated. Entropy at 298.15 K is estimated from that of the component oxides and the difference from the oxides observed for twice $LiBO_2$(cr).

Decomposition Data

The incongruent melting point reported by Sastry and Hummel[4] is used here.

References

[1] L. Shartsis and W. Capps, J. Am. Ceram. Soc. 37, 27 (1954).

[2] JANAF Thermochemical Tables: B_2O_3(l) 12–31–64; Li_2O(cr), 3–31–64.

[3] G. S. Smith, Ph.D. Thesis, Penn. State Univ., Univ. Microfilms, Order No. 59–2916 (1959).

[4] B.S.R. Sastry and F. A. Hummel, J. Am. Ceram. Soc. 42, 216 (1959).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	293.215	188.280	188.280	0.	−4659.888	−4382.421	767.782
300	293.633	190.095	188.286	0.543	−4659.835	−4380.700	762.748
400	316.269	277.724	200.080	31.057	−4657.552	−4288.034	559.960
500	336.561	350.530	223.085	63.723	−4662.433	−4195.190	438.268
600	354.008	413.481	249.687	98.277	−4661.531	−4101.824	357.096
700	368.401	469.162	277.139	134.416	−4660.445	−4008.622	299.127
800	380.493	519.165	304.320	171.876	−4659.158	−3915.591	255.662
900	390.744	564.586	330.753	210.450	−4657.685	−3822.731	221.866
1000	399.572	606.219	356.247	249.972	−4656.018	−3730.046	194.838
1100	406.456	644.627	380.740	290.275	−4654.202	−3637.535	172.732
1200	413.157	680.281	404.234	331.257	−4652.249	−3545.196	154.318
1300	419.675	713.610	426.764	372.900	−4650.116	−3453.027	138.744
1400	426.012	744.944	448.383	415.186	−4647.768	−3361.029	125.402
1500	432.165	774.547	469.149	458.096	−4645.185	−3269.209	113.844
1600	438.137	802.630	489.122	501.613	−4642.361	−3177.568	103.737
1700	443.926	829.367	508.356	545.718	−4929.767	−3071.759	94.384
1800	449.532	854.900	526.905	590.392	−4924.960	−2962.603	85.973
1900	454.956	879.351	544.815	635.618	−4919.944	−2853.719	78.454
2000	460.198	902.822	562.133	681.377	−4914.730	−2745.104	71.695

PREVIOUS: December 1962 CURRENT: March 1965

Sodium Borate ($Na_2B_6O_{10}$) CRYSTAL M_r = 270.83354 Sodium Borate ($Na_2B_6O_{10}$) $B_6Na_2O_{10}$(cr)

$\Delta_f H°$(0 K) = Unknown

$S°$(298.15 K) = [232.2 ± 6.3] J·K^{-1}·mol^{-1}

$\Delta_f H°$(298.15 K) = −4580.48 ± 9.2 kJ·mol^{-1}

T_{dcm} = 1039 K

Enthalpy of Formation

The enthalpy of reaction $Na_2O(cr) + 3\ B_2O_3(l) \rightarrow Na_2B_6O_{10}(cr)$ was reported by Shartsis and Capps[1] from their enthalpy of solution measurements. Their values for the enthalpy of reaction of the oxides have been converted to the enthalpies of formation using JANAF values[2] for B_2O_3(l) and Na_2O(cr). The above $\Delta_f H°$ = −97.52 kcal·mol^{-1}.

Heat Capacity and Entropy

The enthalpy measurements of Smith[3] in the range 298 to 1039 K were smoothed graphically and used to determine C_p. Above this range C_p was extrapolated. Entropy at 298.15 K was estimated as described in detail for $K_2B_6O_{10}$(cr).

Decomposition Data

The incongruent melting point was reported by Morey and Merwin[4] the products are $Na_2B_4O_7$(l) and $Na_2B_8O_{13}$(cr).

References

[1] L. Shartsis and W. Capps, J. Am. Ceram. Soc. 37, 27 (1954).

[2] JANAF Thermochemical Tables: B_2O_3(l), 12–31–64; Na_2O(cr), 6–30–62.

[3] G. S. Smith, Ph.D. Thesis, Penn. State Univ., Univ. Microfilms, Order No. 59–2916 (1959).

[4] G. W. Morey and H. E. Merwin, J. Am. Chem. Soc. 58, 2248 (1936).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	243.509	232.212	232.212	0.	−4580.476	−4302.768	753.827
300	244.346	233.721	232.217	0.451	−4580.527	−4301.045	748.878
400	283.173	309.380	242.270	26.844	−4588.408	−4207.071	549.387
500	319.992	376.581	262.525	57.028	−4590.107	−4111.507	429.526
600	353.757	437.950	286.718	90.739	−4590.114	−4015.757	349.603
700	384.677	494.845	312.434	127.687	−4588.273	−3920.150	292.525
800	412.375	548.063	338.597	167.572	−4584.587	−3824.935	249.743
900	436.182	598.047	364.677	210.033	−4579.219	−3730.284	216.500
1000	456.056	645.071	390.389	254.682	−4572.428	−3636.311	189.941
1100	471.453	689.291	415.572	301.090	−4564.561	−3543.071	168.246
1200	482.917	730.824	440.131	348.831	−4749.519	−3445.703	149.988
1300	491.746	769.840	464.008	397.582	−4738.691	−3337.488	134.102
1400	498.482	806.540	487.177	447.108	−4727.528	−3230.120	120.517
1500	503.461	841.109	509.632	497.217	−4716.188	−3123.559	108.772
1600	507.017	873.720	531.378	547.747	−4704.808	−3017.754	98.520
1700	509.737	904.543	552.431	598.590	−4693.479	−2912.661	89.495
1800	511.829	933.739	572.811	649.672	−4682.263	−2808.233	81.493
1900	513.544	961.459	592.542	700.941	−4671.198	−2704.422	74.350
2000	515 134	987.841	611.653	752.376	−4660.301	−2601.189	67.936

PREVIOUS: March 1963 CURRENT: March 1965

Sodium Borate ($Na_2B_6O_{10}$) $B_6Na_2O_{10}$(cr)

Lead Borate (PbB_6O_{10}) CRYSTAL $M_r = 432.0540$ Lead Borate (PbB_6O_{10}) $B_6O_{10}Pb_1(cr)$

$\Delta_f H°(0\ K)$ = Unknown

$S°(298.15\ K) = [203.3 \pm 13]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_f H°(298.15\ K) = -4197 \pm 8\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

See the $PbB_2O_4(cr)$ table for the complete writeup. Evans[1] analysed the enthalpies of formation of lead borate system based upon Shartsis and Newman's enthalpies of solution and Mazzetti and De Carli's phase studies. From the Shartsis and Newman paper Evans obtained the following:

$$PbO(cr) + 3B_2O_3(cr) \rightarrow PbO.3B_2O_3(gls) \quad \Delta_r H = -24.5\ kcal{\cdot}mol^{-1}$$

and estimated a $\Delta_r H°(298.15\ K)$ of 16.0 $kcal{\cdot}mol^{-1}$ for the conversion to the $PbO{\cdot}3B_2O_3(cr)$. With auxiliary JANAF values the $\Delta_f H°(298.15\ K)$ is calculated to be $-1003.00\ kcal{\cdot}mol^{-1}$.

Heat Capacity and Entropy

The heat capactiy employed in this table was obtained by graphically smoothing the summation of heat capacities of the constituent oxides.

The entropy at 298.15 K was obtained in the manner decribed in the PbB_4O_7 table from $S°(298.15\ K)$ for PbB_4O_7 and B_2O_3 and the subtraction of 4.2 $cal{\cdot}K^{-1}{\cdot}mol^{-1}$.

References

[1] W. H. Evans, U.S. Nat. Bur. Stand., Report 7192, Ch. 6 (July 1, 1961); refer to pp. 80–1.

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	230.957	203.342	203.342	0.	−4196.552	−3921.603	687.049
300	231.794	204.774	203.347	0.428	−4196.572	−3919.897	682.515
400	286.186	279.058	213.108	26.380	−4196.379	−3827.635	499.838
500	334.218	348.197	233.290	57.454	−4193.800	−3735.697	390.266
600	375.849	412.869	257.889	92.988	−4188.839	−3644.504	317.282
700	413.714	473.741	284.419	132.526	−4186.327	−3553.532	265.168
800	444.466	531.083	311.705	175.503	−4176.749	−3463.763	226.161
900	467.060	584.797	339.098	221.129	−4165.426	−3375.304	195.898
1000	483.629	634.906	366.203	268.703	−4152.890	−3288.176	171.757
1100	495.469	681.590	392.778	317.694	−4139.548	−3202.344	152.067
1200	503.000	725.044	418.678	367.640	−4125.774	−3117.750	135.712
1300	507.812	765.511	443.819	418.199	−4111.850	−3034.313	121.920
1400	510.406	803.246	468.160	469.120	−4097.997	−2951.946	110.138
1500	511.787	838.510	491.688	520.234	−4084.360	−2870.563	99.962
1600	512.707	871.570	514.408	571.459	−4071.001	−2790.081	91.087
1700	513.502	902.678	536.342	622.771	−4057.931	−2710.424	83.281
1800	514.130	932.047	557.517	674.154	−4045.156	−2631.531	76.365
1900	514.590	959.857	577.968	725.591	−4032.686	−2553.337	70.196
2000	514.967	986.262	597.728	777.069	−4020.525	−2475.792	64.661

PREVIOUS December 1962   CURRENT March 1965

Potassium Borate ($K_2B_8O_{13}$) CRYSTAL $M_r = 372.6688$

$S°(298.15\ K) = [293.7 \pm 16.7]\ J·K^{-1}·mol^{-1}$
$T_{fus} = 1130\ K$

$\Delta_f H°(0\ K)$ = Unknown
$\Delta_f H°(298.15) = -5945.13 \pm 5.9\ kJ·mol^{-1}$
$\Delta_{fus} H° = 149.8 \pm 4\ kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of reaction $K_2O(cr) + 4\ B_2O_3(l) \rightarrow K_2B_8O_{13}(cr)$ was reported by Shartsis and Capps[1] from their enthalpy of solution measurements. Their values for the enthalpy of reaction of the oxides have been converted to the enthalpies of formation using JANAF values[2] for $B_2O_3(l)$ and $K_2O(cr)$.The above $\Delta_r H° = -137.00\ kcal·mol^{-1}$.

Heat Capacity and Entropy

The enthalpy measurements of Smith[3] in the range 298 to 1130 K were smoothed graphically and used to determine C_p. Above this range C_p is extrapolated.

$S°(298.15\ K)$ is obtained by estimating the entropy of $Na_2B_8O_{13}(cr)$ as $65.7 \pm 2.5\ cal·K^{-1}·mol^{-1}$ as described on the table for $K_2B_6O_{10}(cr)$ and then using an average value of $4.5 \pm 1.5\ cal·K^{-1}·mol^{-1}$ for the replacement of Na_2 by K_2.

Fusion Data

T_{fus} is given by Rollet.[4] $\Delta_{fus} H°$ was obtained from the values of $\Delta_f H°$ for $K_2B_8O_{13}(cr)$ and $K_2B_8O_{13}(l)$ at 298.15 K reported above and the enthalpy of the crystal and liquid at T_{fus}.

References

[1] L. Shartsis and W. Capps, J. Am. Ceram. Soc. 37, 27 (1954).
[2] JANAF Thermochemical Tables: $B_2O_3(l)$, 12–31–64; $K_2O(cr)$, 6–30–63.
[3] G. S. Smith, Ph.D. Thesis, Penn State Univ., Univ. Microfilms, Order No. 59–2916 (1959).
[4] A.–P. Rollet, Comp. rend. **200**, 1763 (1935).

Potassium Borate ($K_2B_8O_{13}$) $B_8K_2O_{13}(cr)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	321.289	293.717	293.717	0.	−5945.129	−5582.653	978.058
300	322.042	295.707	293.723	0.595	−5945.165	−5580.404	971.635
400	360.493	393.657	306.819	34.735	−5952.194	−5457.589	712.688
500	397.313	478.036	332.801	72.617	−5954.258	−5333.683	557.206
600	435.136	553.841	363.420	114.252	−5955.089	−5209.463	453.524
700	471.453	623.739	395.677	159.643	−5954.085	−5085.245	379.466
800	500.406	688.630	428.291	208.272	−5951.363	−4961.293	323.939
900	525.092	749.032	460.612	259.578	−5947.212	−4837.770	280.777
1000	546.012	805.494	492.308	313.186	−5941.830	−4714.777	246.275
1100	560.656	858.271	523.206	368.571	−6093.530	−4583.146	217.635
1130.000	563.825	873.400	532.303	385.440	--- CRYSTAL <--> LIQUID ---		
1200	574.045	907.597	553.205	425.270	−6084.767	−4446.220	193.539
1300	586.178	954.032	582.269	483.292	−6075.326	−4310.053	173.180
1400	597.057	997.879	610.404	542.464	−6065.317	−4174.635	155.758
1500	606.680	1039.407	637.632	602.662	−6054.821	−4039.951	140.684
1600	615.048	1078.835	663.986	663.758	−6043.933	−3905.979	127.517
1700	622.161	1116.342	689.501	725.629	−6032.754	−3772.698	115.921
1800	628.018	1152.075	714.215	788.149	−6021.394	−3640.083	105.632
1900	632.621	1186.159	738.164	851.191	−6009.968	−3508.098	96.444
2000	635.968	1218.699	761.383	914.631	−5998.593	−3376.715	88.191

PREVIOUS: March 1963 CURRENT. March 1965

Potassium Borate ($K_2B_8O_{13}$) LIQUID $M_r = 372.6688$ Potassium Borate ($K_2B_8O_{13}$) $B_8K_2O_{13}(l)$

$S°(298.15\ K) = [302.212]\ J·K^{-1}·mol^{-1}$
$T_{fus} = 1130\ K$

$\Delta_f H°(0\ K) = [-5897.253]\ kJ·mol^{-1}$
$\Delta_{fus} H° = 149.8 \pm 4\ kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of reaction $K_2O(cr) + 4B_2O_3(l) \rightarrow K_2B_8O_{13}(l)$ was reported by Shartsis and Capps[1] their enthalpies of solution measurments. Their values for the enthalpy of reaction of the oxides have been converted to the enthalpies of formation using JANAF values[2] for $B_2O_3(l)$ and for $K_2O(cr)$. The above $\Delta_r H° = -119.65\ kcal·mol^{-1}$.

Heat Capacity and Entropy

The enthalpy measurements of Smith[3] in the range 298 to 1373 K on the glass and liquid were smoothed graphically and used to determine C_p. There is a discontinuity in the C_p curve, a glass transition at about 673 K. Above 673 K the C_p values were estimated to be constant.

The entropy is calculated from that of the crystal by adding $\Delta_{fus}S°$ and differences in entropy, $S°(1130\ K)-S°(298.15\ K)$, between the crystal and liquid.

Fusion Data

Refer to the crystal table for details.

References

[1] L. Shartsis and W. Capps, J. Am. Ceram. Soc. 37, 27 (1954).
[2] JANAF Thermochemical Tables: $B_2O_3(l)$, 12–31–64; $K_2O(cr)$, 6–30–63.
[3] G. S. Smith, Ph.D. Thesis, Penn State Univ., Univ. Microfilms, Order No. 59–2916 (1959).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

		$J·K^{-1}mol^{-1}$		$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0							
100							
200							
250							
298.15	323.088	302.212	302.212	.000	−5897.253	−5537.309	970.114
300	324.511	304.215	302.218	.599	−5897.285	−5535.076	963.742
400	393.798	407.368	315.813	36.622	−5902.431	−5413.311	706.906
500	450.198	501.882	343.717	79.083	−5899.917	−5291.264	552.775
600	475.302	586.656	377.292	125.618	−5895.847	−5169.911	450.081
673.000	473.866	641.307	403.024	160.364	GLASS <--> LIQUID		
673.000	661.490	641.307	403.024	160.364			TRANSITION
700	661.490	667.327	412.720	178.225	−5887.628	−5049.299	376.783
800	661.490	755.657	450.189	244.374	−5867.385	−4930.936	321.957
900	661.490	833.569	488.544	310.523	−5848.391	−4815.032	279.457
1000	661.490	903.264	526.592	376.672	−5830.468	−4701.185	245.565
1100	661.490	966.311	563.746	442.821	−5971.405	−4579.864	217.480
1130.000	661.490	984.110	574.671	462.666	--- CRYSTAL <--> LIQUID ---		
1200	661.490	1023.868	599.726	508 970	−5953.192	−4454.170	193.885
1300	661.490	1076.815	634.416	575.119	−5935.623	−4329.968	173.980
1400	661.490	1125.837	667.789	641.268	−5918.637	−4207.097	156.969
1500	661.490	1171.475	699.864	707.417	−5902.190	−4085.423	142.267
1600	661.490	1214.167	730.688	773.566	−5886.250	−3964.827	129.438
1700	661.490	1254.269	760.319	839.715	−5870.792	−3845.213	118.149
1800	661.490	1292.079	788.821	905.864	−5855.803	−3726.499	108.140
1900	661.490	1327.844	816.258	972.013	−5841.270	−3608.602	99.207
2000	661.490	1361.774	842.693	1038.162	−5827.186	−3491.459	91.188
2100	661 490	1394.048	868.186	1104.311	−5813.546	−3375.010	83.949
2200	661.490	1424.821	892.794	1170.460	−5800.347	−3259.196	77.383
2300	661.490	1454.225	916.569	1236.609	−5787.588	−3143.979	71.402
2400	661.490	1482.378	939.562	1302.758	−6177.341	−3020.757	65.745
2500	661.490	1509.381	961.818	1368.907	−6166.081	−2889.465	60.372
2600	661.490	1535.326	983.381	1435.056	−6154.999	−2758.619	55.421
2700	661.490	1560.290	1004.288	1501.206	−6144.097	−2628.195	50.845
2800	661.490	1584.347	1024.578	1567.355	−6133.377	−2498.171	46.604
2900	661.490	1607.560	1044.283	1633.504	−6122.843	−2368.534	42.662
3000	661.490	1629.985	1063.435	1699.653	−6112.499	−2239.249	38.989

PREVIOUS: March 1963 CURRENT. March 1965

Potassium Borate ($K_2B_8O_{13}$) $B_8K_2O_{13}(l)$

Potassium Borate ($K_2B_8O_{13}$) CRYSTAL-LIQUID

298.15	to 1130 K	crystal
above	1130 K	liquid

Refer to the individual tables for details.

M_r = 372.6688 Potassium Borate ($K_2B_8O_{13}$) $B_8K_2O_{13}$(cr,l)

Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	321.289	293.717	293.717	0.	−5945.129	−5582.653	978.058
300	322.042	295.707	293.723	0.595	−5945.165	−5580.404	971.635
400	360.493	393.657	306.819	34.735	−5952.194	−5457.589	712.688
500	397.313	478.036	332.801	72.617	−5954.258	−5333.683	557.206
600	435.136	553.841	363.420	114.252	−5955.089	−5209.463	453.524
700	471.453	623.739	395.677	159.643	−5954.085	−5085.245	379.466
800	500.406	688.630	428.291	208.272	−5951.363	−4961.293	323.939
900	525.092	749.032	460.612	259.578	−5947.212	−4837.770	280.777
1000	546.012	805.494	492.308	313.186	−5941.830	−4714.777	246.275
1100	560.656	858.271	523.206	368.571	−6093.530	−4583.146	217.635
1130.000	563.825	873.400	532.303	385.440	CRYSTAL <--> LIQUID		
1130.000	661.490	1005.983	532.303	535.258	TRANSITION		
1200	661.490	1023.868	559.830	556.846	−5953.192	−4454.170	193.885
1300	661.490	1076.815	597.589	622.995	−5935.623	−4329.968	173.980
1400	661.490	1125.837	633.591	689.144	−5918.637	−4207.097	156.969
1500	661.490	1171.475	667.947	755.293	−5902.190	−4085.422	142.267
1600	661.490	1214.167	700.766	821.442	−5886.250	−3964.827	129.438
1700	661.490	1254.269	732.157	887.591	−5870.792	−3845.213	118.149
1800	661.490	1292.079	762.224	953.740	−5855.803	−3726.499	108.140
1900	661.490	1327.844	791.060	1019.889	−5841.270	−3608.602	99.207
2000	661.490	1361.774	818.755	1086.038	−5827.186	−3491.458	91.188
2100	661 490	1394.048	845.388	1152.187	−5813.546	−3375.009	83.949
2200	661.490	1424.821	871.032	1218.336	−5800.347	−3259.196	77.383
2300	661.490	1454.225	895.753	1284.485	−5787.588	−3143.979	71.402
2400	661.490	1482.378	919.614	1350.634	−6177.341	−3020.757	65.745
2500	661.490	1509.381	942.668	1416.783	−6166.081	−2889.464	60.372
2600	661.490	1535.326	964.967	1482.932	−6154.999	−2758.619	55.421
2700	661.490	1560.290	986.557	1549.081	−6144.097	−2628.194	50.845
2800	661.490	1584.347	1007.479	1615.230	−6133.377	−2498.171	46.604
2900	661.490	1607.560	1027.774	1681.379	−6122.843	−2368.534	42.662
3000	661.490	1629.985	1047.476	1747.529	−6112.499	−2239.249	38.989

PREVIOUS: CURRENT: March 1965

Potassium Borate ($K_2B_8O_{13}$) $B_8K_2O_{13}$(cr,l)

Lithium Borate ($Li_2B_8O_{13}$) CRYSTAL M_r = 308.3542 Lithium Borate ($Li_2B_8O_{13}$) $B_8Li_2O_{13}$(cr)

$S°(298.15\ K) = [265.3 \pm 4]\ J \cdot K^{-1} \cdot mol^{-1}$
$T_{dcm} = 908 \pm 10\ K$

$\Delta_f H°(0\ K)$ = Unknown
$\Delta_f H°(298.15) = -5914.38 \pm 6.8\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The enthalpy of the reaction $Li_2O(cr) + 4\ B_2O_3(l) \rightarrow Li_2B_8O_{13}(cr)$ was reported by Shartsis and Capps[1] from their enthalpy of solution measurements. Their values for the enthalpy of reaction of the oxides have been converted to the enthalpies of formation using JANAF values[2] for $B_2O_3(l)$ and for $Li_2O(cr)$. The above $\Delta_r H° = -73.35\ kcal \cdot mol^{-1}$.

Heat Capacity and Entropy

The enthalpy measurements of Smith[3] in the range 298 to 823 K were used to determine C_p. Above this range C_p is extrapolated. The entropy at 298.15 K is estimated from that of the component oxides and the difference from the oxides observed for twice $LiBO_2$(cr).

Decomposition Data

The incongruent melting point reported by Sastry and Hummel[4] is used here.

References

[1] L. Shartsis and W. Capps, J Am. Ceram. Soc. 37, 27 (1954).
[2] JANAF Thermochemical Tables: B_2O_3(l), 12–31–64; Li_2O(cr), 3–31–64.
[3] G. S. Smith, Ph.D. Thesis, Penn State Univ., Univ. Microfilms, Order No. 59–2916 (1959).
[4] B. S. R. Sastry and T. A. Hummel, J. Am. Ceram. Soc. 42, 216 (1959).

Enthalpy Reference Temperature = T_r = 298.15 K — Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	325.515	265.266	265.266	0.	−5914.377	−5564.637	974.901
300	326.770	267.283	265.272	0.603	−5914.386	−5562.467	968.512
400	390.367	370.606	278.926	36.672	−5913.731	−5445.208	711.071
500	428.567	462.069	306.606	77.732	−5918.268	−5327.630	556.574
600	453.211	542.480	339.359	121.873	−5916.480	−5209.666	453.542
700	471.537	613.760	373.565	168.137	−5914.462	−5092.021	379.971
800	486.683	677.748	407.656	216.074	−5912.270	−4974.678	324.813
900	498.733	735.788	440.941	265.362	−5909.954	−4857.617	281.929
1000	508.649	788.860	473.117	315.743	−5907.545	−4740.819	247.635
1100	517.142	837.742	504.072	367.037	−5905.062	−4624.264	219.588
1200	524.623	883.062	533.789	419.127	−5902.502	−4507.941	196.226
1300	531.915	925.343	562.300	471.956	−5899.841	−4391.835	176.466
1400	539.016	965.023	589.664	525.504	−5897.031	−4275.938	159.537
1500	545.928	1002.448	615.947	579.752	−5894.040	−4160.251	144.873
1600	552.651	1037.897	641.221	634.683	−5890.855	−4044.767	132.048
1700	559.183	1071.599	665.554	690.276	−6177.943	−3915.137	120.298
1800	565.526	1103.741	689.012	746.513	−6172.856	−3782.179	109.756
1900	571.679	1134.483	711.654	803.375	−6167.596	−3649.505	100.332
2000	577.643	1163.959	733.538	860.843	−6162.172	−3517.113	91.858

PREVIOUS: December 1962 CURRENT March 1965

Decaborane ($B_{10}H_{14}$) CRYSTAL $M_r = 122.21116$

$S°(298.15\ K) = 176.56\ J \cdot K^{-1} \cdot mol^{-1}$

$T_{fus} = 371.93\ K$

$\Delta_f H°(0\ K) = 14.3 \pm 19\ kJ \cdot mol^{-1}$

$\Delta_f H°(298.15) = -28.9 \pm 19\ kJ \cdot mol^{-1}$

$\Delta_{fus} H° = 21.966 \pm 0.04\ kJ \cdot mol^{-1}$

Enthalpy of Formation

The enthalpy change of the reaction $B_{10}H_{14}(cr) \rightarrow 10\ B(am) + 7H_2(g)$ was reported to be 19.8 ± 1.4 and 18.0 ± 1.0 kcal·mol^{-1} by Johnson, Kilday and Prosen[1] and Gal'chenko, Timofeev and Skuratov,[2] respectively Using $\Delta_r H°(298.15\ K) = 1.2 \pm 0.4$ kcal·mol^{-1} for the reaction $B(cr) \rightarrow B(am)$, the corresponding $\Delta_f H°(298.15\ K)$ values for $B_{10}H_{14}(cr)$ are calculated to be −7.8 and −6.0 kcal·mol^{-1}. The adopted value $\Delta_f H°(298.15\ K)$ for $B_{10}H_{14}(cr)$ is the average of these two.

Heat Capacity and Entropy

C_p(60 to 371.93 K) was given by Furukawa and Park.[3] The heat capacity above 371.93 K is estimated by comparison with that of the liquid decarborane. Heat capacity (14 to 205 K) was also reported by Kerr, Hallett and Johnston.[4] The value of $S°(298.15\ K)$ was taken from Furukawa and Park.[3]

Fusion Data

T_{fus} and $\Delta_{fus}H°$ were obtained from Furukawa and Park.[3]

Sublimation Data

$\Delta_{sub}H°(298.15\ K)$ is calculated from Gibbs energy functions and vapor pressure reported by Furukawa and Park.[3] Refer to the ideal gas table for details.

References

[1] W. H. Johnson, M. V. Kilday, and E. J. Prosen, J. Res. Nat. Bur. Stand. **64A**, 521 (1960).

[2] G. L. Gal'chenko, B. I. Timofeev, and S. M. Skuratov, Dokl. Akad. Nauk SSSR **142**, 1077 (1962).

[3] G. T. Furukawa and R. P. Park, J. Res. Nat. Bur. Stand. **55**, 255 (1955).

[4] E. C. Kerr, N. C. Hallett, and H. L. Johnston, J. Am. Chem, Soc. **73**, 1117 (1951).

Decaborane ($B_{10}H_{14}$) $B_{10}H_{14}(cr)$

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−28.292	14.248	14.248	INFINITE
100	55.580	53.212	305.968	−25.276	−3.969	61.527	−32.138
200	123.386	109.725	193.426	−16.740	−17.619	132.450	−34.592
298.15	217.953	176.565	176.565	0.	−28.870	208.617	−36.549
300	219.706	177.918	176.569	0.405	−29 048	210.091	−36.580
371.930	293 483	232.548	182.044	18.784	--- CRYSTAL <--> LIQUID ---		
400	305.014	254.416	186.360	27.222	−36.197	291.017	−38.003
500	326.352	324.505	207.161	58.672	−42.516	373.532	−39.023
600	364.845	387.498	232.030	93.281	−48.223	457.307	−39.812
700	397.480	446.265	258 485	131.446	−52.174	541.898	−40.437
800	421.538	500.946	285.418	172.423	−54.694	626.951	−40.936
900	442.458	551.835	312.225	215.649	−56.109	712.253	−41.338
1000	460.240	599.400	338.590	260.810	−56.596	797.660	−41.665
1100	474.884	643.978	364.348	307.592	−56.385	883.080	−41.934
1200	486.390	685.814	389.412	355 682	−55.733	968 459	−42.156
1300	494.758	725 097	413.739	404 766	−54.909	1053.776	−42.341
1400	499.988	761.974	437.310	454.529	−54.192	1139 030	−42.498
1500	502.080	796.559	460.119	504 659	−53.862	1224.246	−42.632

PREVIOUS: September 1962 CURRENT: December 1964

Decaborane ($B_{10}H_{14}$) $B_{10}H_{14}(cr)$

Decaborane ($B_{10}H_{14}$) LIQUID M_r = 122.21116 Decaborane ($B_{10}H_{14}$) $B_{10}H_{14}(l)$

$S°(298.15\ K) = [234.935]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 371.93\ K$

$\Delta_f H°(298.15\ K) = [-7.133]\ kJ{\cdot}mol^{-1}$
$\Delta_{fus}H° = 21.966 \pm 0.04\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(B_{10}H_{14}$, cl, 298.15 K) is calculated from $\Delta_f H°(B_{10}H_{14}$, cr, 298.15 K), by adding $\Delta_{fus}H°$ reported by and Park[1] and the enthalpy difference, $H°(371.93\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

C_p (371.93 to 380 K) was measured by Furukawa and Park.[1] Heat capacities below 371.93 and above 380 K were estimated by comparison with that of the gaseous decarborane. $S°(298.15\ K)$ is calculated from that of crystal in a manner analogous to the used for the enthalpy of formation.

Fusion and Vaporization Data

T_{fus} and $\Delta_{fus}H°$ were obtained from Furukawa and Park.[1] T_{vap} and $\Delta_{vap}H°$ are calculated from functions for $B_{10}H_{14}(l)$ and $B_{10}H_{14}(g)$.

References

[1] G. T Furukawa and R. P. Park, J. Res. Nat. Bur. Stand, 55, 255 (1955).

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	221.208	234.935	234.935	0.	−7.133	212.950	−37.308
300	222.924	236.309	234.939	0.411	−7.305	214.316	−37.316
371.930	296.720	291.607	240.487	19.013	--- CRYSTAL <--> LIQUID ---		
400	323.005	314.790	244.892	27.959	−13.724	289.341	−37.784
500	347.272	389.393	266.520	61.436	−18.015	365.589	−38.193
600	389.949	456.569	292.659	98.346	−21.421	442.666	−38.538
700	426.768	519.520	320.619	139.231	−22.652	520.141	−38.813
800	456.056	578.465	349.207	183.407	−21.973	597.656	−39.023
900	481.160	633.672	377.780	230.302	−19.718	674.990	−39.175
1000	502.080	685.486	405.987	279.499	−16.169	752.000	−39.280
1100	518.816	734.158	433.631	330.579	−11.661	828.605	−39.347
1200	531.368	779.869	460.600	383.123	−6.555	904.771	−39.384
1300	539.736	822.760	486.826	436.713	−1.225	980.499	−39.397
1400	543.920	862.937	512.272	490.931	3.947	1055.820	−39.393
1500	543.920	900.488	536.916	545.358	8.574	1130.788	−39.378

PREVIOUS: September 1962 CURRENT: December 1964

Decaborane ($B_{10}H_{14}$) $B_{10}H_{14}(l)$

Decaborane ($B_{10}H_{14}$) CRYSTAL-LIQUID

0 to 371.93 K crystal
above 371.93 K liquid

Refer to the individual tables for details.

M_r = 122.21116 Decaborane ($B_{10}H_{14}$) $B_{10}H_{14}$(cr,l)

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−28.292	14.248	14.248	INFINITE
100	55.580	53.212	305.968	−25.276	−3.969	61.527	−32.138
200	123.386	109.725	193.426	−16.740	−17.619	132.450	−34.592
298.15	217.953	176.565	176.565	0.	−28.870	208.617	−36.549
300	219.706	177.918	176.569	0.405	−29.048	210.091	−36.580
371.930	293.483	232.548	182.044	18.784	CRYSTAL <--> LIQUID		
371.930	296.720	291.607	182.044	40.750	TRANSITION		
400	323.005	314.790	190.551	49.696	−13.724	289.340	−37.784
500	347.272	389.393	223.047	83.173	−18.015	365.589	−38.193
600	389.949	456.569	256.431	120.083	−21.421	442.666	−38.537
700	426.768	519.520	289.567	160.967	−22.653	520.141	−38.813
800	456.056	578.465	322.036	205.143	−21.973	597.656	−39.023
900	481.160	633.672	353.628	252.039	−19.718	674.990	−39.175
1000	502.080	685.486	384.250	301.236	−16.170	752.000	−39.280
1100	518.816	734.158	413.871	352.316	−11.661	828.605	−39.347
1200	531.368	779.869	442.486	404.860	−6.555	904.771	−39.384
1300	539.736	822.760	470.106	458.450	−1.225	980.499	−39.397
1400	543.920	862.937	496.746	512.667	3.946	1055.819	−39.393
1500	543.920	900.488	522.425	567.094	8.574	1130.787	−39.378

PREVIOUS: CURRENT: December 1964

Decarborane ($B_{10}H_{14}$) IDEAL GAS M_r = 122.21116 Decaborane (B_9H_{14}) $B_{10}H_{14}(g)$

$S°(298.15\ K) = 352.16\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 93.8 \pm 18.8\ kJ{\cdot}mol^{-1}$

$\Delta_fH°(298.15\ K) = 47.3 \pm 18.8\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies
υ, cm $^{-1}$

230(1)	295(1)	344(1)	350(1)	387(1)	434(1)	446(1)	452(1)
464(1)	508(1)	588(1)	618(1)	635(1)	651(1)	690(1)	701(1)
709(1)	720(1)	747(1)	752(1)	767(1)	773(1)	814(1)	822(1)
832(1)	859(1)	862(1)	903(1)	915(1)	921(1)	924(1)	938(1)
942(1)	960(1)	967(1)	972(1)	1008(1)	1037(1)	1060(1)	1104(1)
1160(1)	1190(1)	1210(1)	1250(1)	1300(1)	1360(1)	1104(1)	1410(1)
1460(1)	1500(1)	1555(1)	1590(1)	1620(1)	1665(1)	1880(2)	1929(2)

Ground State Quantum Weight: [1] $\sigma = 2$

Point Group: C_{2v}

Bond Distances: B–B = 1.762 Å; B–B(apex) = 1.773 Å
B–H(bridge) = 1.394 Å; B–H = 1.256 Å

Bond Angles: B–B–B = 108°; H–B(apex)–B = 59° 34'; B–B–B(apex) = 60° 13'
B–H(bridge)–B = 46° 17'; B(apex–B–H) = 87° 42'; B(center)–B(center)–H = 120°

Product of the Moments of Inertia: $I_AI_BI_C = 8.657643 \times 10^{-113}\ g^3{\cdot}cm^6$

Enthalpy of Formation

The vapor pressures of decaborane were measured by Furukawa and Park[1] and Miller.[2] The enthalpies of vaporization were derived by both the 2nd and 3rd law methods. Using the average value of $\Delta_{vap}H°$, the respective of enthalpies of formation for $B_{10}H_{14}(g)$ are calculated.

Source	Reaction	$\Delta_vH°(298.15)$, $kcal{\cdot}mol^{-1}$ 2nd law	3rd law	$\Delta_fH°(298.15)$ $kcal{\cdot}mol^{-1}$
1	$B_{10}H_{14}(cr) \rightarrow B_{10}H_{14}(g)$	16.63 ± 0.93	18.20	10.52 ± 4.5
	$B_{10}H_{14}(l) \rightarrow B_{10}H_{14}(g)$	13.28 ± 0.06	13.06	11.47 ± 4.5
2	$B_{10}H_{14}(cr) \rightarrow B_{10}H_{14}(g)$	17.81 ± 0.01	18.27	11.14 ± 4.5

The adopted value of $\Delta_fH°(298.15\ K)$ for $B_{10}H_{14}(g)$ is the weighted average of the three $\Delta_fH°(298.15\ K)$ values listed in the above table.

Heat Capacity and Entropy

The molecular structure of $B_{10}H_{14}(c)$ were reported by Kasper, Lucht and Harker,[3] Moore, Dickerson, and Lipscomb,[4] and Lipscomb.[5] For the calculation of the moments of inertia for $B_{10}H_{14}(g)$ a simplified molecular model is adopted. The molecule is assumed to be composed of two regular pentagonal pyramids with a common base edge. The angle between the base planes of those pyramids is 73° 30'. Each of 10 H atoms is attached to a single B atom above the base plane. The remaining 4 H atoms, each bridge two B atoms. The vibrational frequencies were obtained from Evans,[6] which were derived based on the infrared and Raman spectra reported by Stewart[7] and Keller and Johnston.[8] The principal moments of inertia are: $I_A = 35.1322 \times 10^{-39}$, $I_B = 45.3594 \times 10^{-39}$, and $I_C = 54.3284 \times 10^{-39}\ g{\cdot}cm^2$.

References

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Enthalpy Reference Temperature = T_r = 298.15 K   Standard State Pressure = $p°$ = 0.1 MPa

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−24.839	93.850	93.850	INFINITE
100	46.005	248.258	460.646	−21.239	76.216	122.208	−63.835
200	105.137	296.347	366.164	−13.963	61.306	174.051	−45.457
250	142.942	323.835	354.911	−7.769	54.016	203.084	−42.432
298.15	179.581	352.159	352.159	0.	47.279	232.412	−40.718
300	180.961	353.275	352.163	0.333	47.029	233.561	−40.667
350	216.949	383.907	354.500	10.292	40.573	265.169	−39.574
400	249.946	415.066	360.121	21.978	34.707	297.661	−38.871
450	279.729	446.256	367.960	35.233	29.462	330.852	−38.404
500	306.427	477.136	377.337	49.900	24.860	364.593	−38.089
600	351.663	537.156	399.010	82.888	17.533	433.268	−37.719
700	387.932	594.191	422.857	119.934	12.463	502.987	−37.533
800	417.186	647.970	447.669	160.241	9.273	573.299	−37.433
900	440.941	698.527	472.762	203.188	7.580	643.918	−37.372
1000	460.360	746.023	497.738	248.285	7.028	714.660	−37.330
1100	476.345	790.674	522.360	295.146	7.318	785.416	−37.296
1200	489.595	832.708	546.488	343.463	8.197	856.117	−37.266
1300	500.656	872.346	570.044	392.992	9.466	926.728	−37.236
1400	509.954	909.799	592.987	443.536	10.963	997.231	−37.207
1500	517.824	945.258	615.301	494.935	12.564	1067.623	−37 178
1600	524.530	978.897	636.983	547.062	14.169	1137.907	−37 149
1700	530.279	1010.873	658.044	599.809	15.700	1208.094	−37 120
1800	535.238	1041.327	678.498	653.091	17.099	1278.193	−37.092
1900	539.541	1070.384	698.365	706.835	18.318	1348.219	−37.065
2000	543.294	1098.156	717.666	760.981	19.318	1418.188	−37.039
2100	546.584	1124.745	736.422	815.479	20.073	1488.112	−37.015
2200	549.483	1150.240	754.656	870.285	20.557	1558.005	−36.992
2300	552.049	1174.723	772.391	925.364	20.752	1627.884	−36.970
2400	554.329	1198.268	789.649	980.685	−481.950	1708.449	−37.183
2500	556.363	1220.938	806.450	1036.222	−483.155	1799.741	−37.604
2600	558.185	1242.795	822.814	1091.951	−484.360	1891.079	−37.992
2700	559.824	1263.893	838.762	1147.853	−485.577	1982.465	−38.353
2800	561.301	1284.279	854.312	1203.910	−486.816	2073.897	−38.689
2900	562.638	1304.000	869.480	1260.108	−488.084	2165.374	−39.003
3000	563.852	1323.095	884.284	1316.434	−489.389	2256.895	−39.296
3100	564.956	1341.602	898.739	1372.875	−490.738	2348.459	−39.571
3200	565.964	1359.555	912.860	1429.422	−492.135	2440.067	−39.830
3300	566.886	1376.985	926.662	1486.065	−493.585	2531.722	−40.074
3400	567.732	1393.921	940.157	1542.796	−495.094	2623.420	−40.304
3500	568.510	1410.389	953.358	1599.609	−496.665	2715.164	−40.522
3600	569.226	1426.415	966.277	1656.496	−498.303	2806.953	−40.728
3700	569.887	1442.020	978.925	1713.452	−500.009	2898.790	−40.924
3800	570.499	1457.226	991.313	1770.472	−501.788	2990.673	−41.110
3900	571.066	1472.053	1003.450	1827.551	−503.643	3082.604	−41.287
4000	571.593	1486.518	1015.347	1884.684	−505.575	3174.582	−41.456
4100	572.082	1500.638	1027.011	1941.868	−507.587	3266.612	−41 617
4200	572.538	1514.429	1038.453	1999.099	−5308.175	3428.933	−42.645
4300	572.964	1527.906	1049.680	2056.375	−5299.480	3636.856	−44.179
4400	573.362	1541.083	1060.699	2113.691	−5290.888	3844.578	−45.641
4500	573.734	1553.972	1071.518	2171.046	−5282.400	4052.105	−47.036
4600	574.083	1566.586	1082.143	2228.437	−5274.020	4259 446	−48.368
4700	574.411	1578.936	1092.582	2285.862	−5265.751	4466.606	−49 641
4800	574.718	1591.033	1102.841	2343.319	−5257.594	4673.594	−50.859
4900	575.008	1602.886	1112.926	2400.805	−5249.551	4880 407	−52.026
5000	575.280	1614.505	1122.842	2458.320	−5241.623	5087.063	−53.144
5100	575.537	1625.900	1132.594	2515.861	−5233.812	5293.556	−54.217
5200	575.780	1637.078	1142.189	2573.427	−5226.117	5499.902	−55.247
5300	576.010	1648.048	1151.630	2631.016	−5218.540	5706 099	−56.237
5400	576.227	1658.817	1160.923	2688.628	−5211.080	5912.155	−57 189
5500	576.432	1669.392	1170.072	2746.261	−5203.735	6118 070	−58 105
5600	576.627	1679.780	1179.081	2803.914	−5196.507	6323.857	−58.987
5700	576.812	1689.988	1187.955	2861.586	−5189.393	6529.516	−59.836
5800	576.987	1700.021	1196.698	2919.276	−5182.391	6735.050	−60.656
5900	577.154	1709.886	1205.313	2976.983	−5175.501	6940.461	−61.446
6000	577.312	1719.588	1213.803	3034.707	−5168.720	7145.758	−62.209

PREVIOUS· December 1964 (1 atm)   CURRENT December 1964 (1 bar)

Decaborane ($B_{10}H_{14}$) $B_{10}H_{14}(g)$

Lead Borate ($Pb_2B_{10}O_{17}$) CRYSTAL $M_r = 794.4898$ Lead Borate ($Pb_2B_{10}O_{17}$) $B_{10}O_{17}Pb_2(cr)$

$\Delta_f H°(0\ K)$ = Unknown

$S°(298.15\ K)$ = [352.7 ± 13] $J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_f H°(298.15)$ = −7087.7 ± 13 $kJ \cdot mol^{-1}$

Enthalpy of Formation

Refer to the $PbB_2O_4(cr)$ table for the complete writeup. Evans[1] analysed the enthalpies of formation of lead borate system based upon Shartsis and Newman's enthalpies of solution and Mazzetti and DeCarli's phase studies. From the Shartsis and Newman paper Evans obtained the following:

$$2\ PbO(cr) + 5\ B_2O_3(cr) \rightarrow 2\ PbO \cdot 5B_2O_3(gls) \quad \Delta_r H = -45.2\ kcal \cdot mol^{-1}$$

and estimated a ΔH_{298} of 26.8 $kcal \cdot mol^{-1}$ for the conversion to the $2PbO \cdot 5B_2O_3(cr)$. With auxiliary JANAF values the $\Delta_f H°(298.15\ K)$ is calculated to be −1694 00 $kcal \cdot mol^{-1}$.

Heat Capacity and Entropy

The heat capacity employed in this table was obtained by graphically smoothing the summation of the heat capacities of the constituent oxides.

The entropy at 298.15 K was obtained in the manner described in the PbB_4O_7 table from the entropies of $PbO \cdot 2B_2O_3$ and $Pb \cdot 3B_2O_3$ and the subtraction of 4.2 $cal \cdot K^{-1} \cdot mol^{-1}$.

References

[1] W. H. Evans, U.S. Nat. Bur. Stand. Report 7192, Ch. 6 (July 1, 1961), refer to pp. 80–1.

Enthalpy Reference Temperature = T_r = 298.15 K Standard State Pressure = $p°$ = 0.1 MPa

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	406.685	352.711	352.711	0.	−7087.696	−6616.932	1159.259
300	408.358	355.232	352.719	0.754	−7087.714	−6614.011	1151.602
400	502.917	486.150	369.928	46.489	−7086.317	−6456.200	843.093
500	576.974	606.499	405.379	100.560	−7081.183	−6299.195	658.072
600	641.826	717.604	448.275	161.597	−7072.593	−6143.547	534.843
700	694.962	820.629	494.201	228.499	−7070.549	−5987.999	446.830
800	740.568	916.489	541.065	300.339	−7055.936	−5834.313	380.942
900	778.642	1005.987	587 807	376.362	−7038.648	−5682.623	329.811
1000	809.186	1089.665	633.856	455.809	−7019.159	−5532.980	289.013
1100	833.034	1167.960	678.891	537.976	−6997.967	−5385.374	255.730
1200	850.189	1241.225	722.733	622.189	−6975.596	−5239.755	228.081
1300	861.067	1309.734	765.282	707 787	−6952.611	−5096.032	204.761
1400	867.762	1373.811	806.485	794.256	−6929.479	−4954.086	184.839
1500	871.109	1433.795	846.328	881.200	−6906.558	−4813.790	167.631
1600	874.456	1490.122	884.823	968.478	−6883.959	−4675.011	152.623
1700	877.803	1543.236	922.005	1056.091	−6861.659	−4537.635	139.425
1800	881.150	1593.504	957.927	1144.039	−6839.645	−4401.567	127.730
1900	884.498	1641.235	992.645	1232.321	−6817.903	−4266.712	117.300
2000	887.845	1686.689	1026.220	1320.938	−6796.422	−4132.994	107.943

PREVIOUS: December 1962 CURRENT: March 1965

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There have been no measurements reported for HBO which provide direct experimental information on its structure. However, the millimeter-wave spectra of the related species HBS[14] have been observed. These results show that this molecule is linear and has a B–S bond length which is 0.01 Å less than that for BS.[1] We assume a similar decrease in r_e(B=O) for the HBO–BO pair, and we obtain r_e(HB–O) = 1.19 Å with r_e(B=O) = 1.20 Å.[1] The H–B bond length is assumed the same as that for HBS.[14] Ab- initio calculations[8] of bond lengths for HBO by an optimization procedure predict values only slightly lower (~0.01 Å) than our estimates. We note that bond lengths computed by this procedure are normally slightly lower (~0.005 Å) than the true values as indicated by the results for HCP[16] and HBS.[17] By analogy with HBS,[14] we assume HBO to be linear. This assumption is in agreement with predictions from the Walsh diagram[15] for HAB molecules with ten valence electrons. In direct evidence available from product rule calculations[2] also tend to support a linear configuration.

References

[1] JANAF Thermochemical Tables: H_2(g), 3–31–61; B_2O_3(l), 6–30–71, BO(g), 6–30–68; B_2O_2(g) and BH_3(g), 12–31–64, HCP(g) and HCN(g), 12–31–69; BS(g), 6–30–72.

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calculation on HCN led these workers to conclude that their ν_2 values were probably lower (~50 cm^{-1}) than the true values They suggested a better estimate of ν_2 as 690 ± 30 cm^{-1}. Pearson and McCormick[8] estimated ν_2 = 680 cm^{-1} from the l-doubling constant determined from their microwave measurements. These latter two values support our selection of ν_2 = 715 cm^{-1}. Photoelectron spectrometric results[10, 11] have led to predictions of ν_3 = 1100 cm^{-1} from the changes observed in vibrational frequencies produced upon ionization. We believe our calculated frequencies are uncertain to no more than ±50 cm^{-1} which amounts to an $S°$(298.15 K) error of ± 0.1 $cal \cdot K^{-1} \cdot mol^{-1}$.

Evidence is available which suggests that the ground state configuration and excited states of HBS are similar to those for the isoelectronic molecule HCP. Theoretical calculations[7, 12] predict the same ordering of valence orbitals for these two molecules. This orbital order is corroborated by the results[10, 11 and 13] of photoelectron spectroscopy where the similarity[11] in their PE spectra has been noted. In addition, we note that the Zeeman parameters recently reported for HBS and HCP by Pearson *et al.*[14] are nearly identical. We assume the same ground state configuration ($^1\Sigma^+$) for HBS as that for HCP,[3] and we estimate the electronic levels by analogy with those observed for HCP.

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