

Potassium (K)

$A_r = 39.0983$ Potassium (K)

$K_1(\text{ref})$

REFERENCE STATE

0 to 336.35 K crystal
 336.35 to 1039.540 K liquid
 above 1039.540 K ideal monatomic gas

Refer to the individual tables for details.

T/K	C_p^0	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa		$\log K_f$
		$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0	INFINITE	-7.082	0	0	0
100	24.631	35.603	-5.350	0	0	0
200	27.004	53.493	-2.755	0	0	0
298.15	29.497	64.670	0	0	0	0
300	29.573	64.853	0.055	0	0	0
336.350	34.567	68.370	1.174	CRYSTAL \leftrightarrow LIQUID	TRANSITION	—
336.350	32.139	75.310	3.508	0	0	0
400	31.489	80.825	5.533	0	0	0
500	30.695	87.765	8.641	0	0	0
600	30.136	93.306	11.680	0	0	0
700	29.824	97.925	14.676	0	0	0
800	29.757	101.901	17.653	0	0	0
900	29.956	105.413	20.636	0	0	0
1000	30.361	108.587	23.648	0	0	0
1039.540	30.604	109.769	24.854	LIQUID \leftrightarrow IDEAL GAS	FUGACITY = 1 bar	—
1039.540	20.786	186.500	104.410	0	0	0
1100	20.786	187.475	105.667	0	0	0
1200	20.787	189.284	107.746	0	0	0
1300	20.789	190.948	109.825	0	0	0
1400	20.793	192.488	111.904	0	0	0
1500	20.801	193.923	113.983	0	0	0
1600	20.814	195.266	116.064	0	0	0
1700	20.836	196.529	118.146	0	0	0
1800	20.868	197.720	120.231	0	0	0
1900	20.914	198.850	122.320	0	0	0
2000	20.975	199.924	124.415	0	0	0
2100	21.056	200.949	126.516	0	0	0
2200	21.157	201.931	128.627	0	0	0
2300	21.281	202.874	130.748	0	0	0
2400	21.431	203.783	132.884	0	0	0
2500	21.606	204.661	135.035	0	0	0
2600	21.809	205.512	137.200	0	0	0
2700	22.043	206.340	139.388	0	0	0
2800	22.307	207.146	141.613	0	0	0
2900	22.605	207.934	143.881	0	0	0
3000	22.936	208.706	146.197	0	0	0
3100	23.306	209.464	148.449	0	0	0
3200	23.714	210.210	150.600	0	0	0
3300	24.123	210.943	152.684	0	0	0
3400	24.599	211.670	154.619	0	0	0
3500	25.107	212.390	156.418	0	0	0
3600	25.666	213.105	158.083	0	0	0
3700	26.270	213.816	159.698	0	0	0
3800	26.920	214.526	161.236	0	0	0
3900	27.618	215.234	162.696	0	0	0
4000	28.345	215.940	164.082	0	0	0
4100	29.124	216.649	165.414	0	0	0
4200	29.962	217.361	166.700	0	0	0
4300	30.848	218.076	167.941	0	0	0
4400	31.145	218.726	169.131	0	0	0
4500	32.003	219.436	170.276	0	0	0
4600	32.892	220.149	171.381	0	0	0
4700	33.767	220.861	172.446	0	0	0
4800	34.664	221.553	173.466	0	0	0
4900	35.383	222.273	174.446	0	0	0
5000	36.319	222.997	175.381	0	0	0
5100	37.263	223.725	176.276	0	0	0
5200	38.212	224.458	177.137	0	0	0
5300	39.165	225.195	177.961	0	0	0
5400	40.111	225.936	178.756	0	0	0
5500	41.052	226.681	179.526	0	0	0
5600	41.980	227.429	180.266	0	0	0
5700	42.477	228.111	180.981	0	0	0
5800	43.337	228.857	181.666	0	0	0
5900	44.172	229.605	182.326	0	0	0
6000	44.978	230.354	182.966	0	0	0

PREVIOUS: December 1961 (1 atm)

CURRENT: December 1961 (1 bar)

Potassium (K)

$K_1(\text{ref})$

K₁(cr)

Potassium (K)

A₁ = 39.0983

CRYSTAL

Potassium (K)

$S^{\circ}(298.15 \text{ K}) = 64.67 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $T_{\text{fus}} = 336.35 \text{ K}$
 $\Delta H^{\circ}(0 \text{ K}) = 0 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_1 H^{\circ}(298.15 \text{ K}) = 0 \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{fus}} H^{\circ} = 2.334 \text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

Low temperature heat capacity measurements have been reported by Roberts (1.5–20 K),¹ Krier, Craig, and Wallace (12–320 K),² Dauphinee, Martin, and Preston Thomas (20–330 K),³ Simon and Zeldler (15–300 K),⁴ and Eastman and Rodebush, (70–290 K).⁵ A smooth curve was drawn through a large scale plot of the data, giving the most weight to the first three references. Above 300 K, the heat capacity data were adjusted to join smoothly with the enthalpy measurements of Douglas *et al.*⁶

Fusion DataThe enthalpy of fusion is from the enthalpy measurements of Douglas *et al.*⁶**Sublimation Data**Refer to the K(g) and K₂(g) tables for details.**References**

- ¹L. M. Roberts, Proc. Phys. Soc. (London) 70B, 744 (1957).
- ²C. A. Krier, R. S. Craig, and W. E. Wallace, J. Phys. Chem. 61, 522 (1957).
- ³T. M. Dauphinee, D. L. Martin, and H. Preston Thomas, Proc. Roy. Soc. (London) A233, 214 (1955).
- ⁴F. Simon and W. Zeldler, Z. Physik. Chem. 123, 383 (1926).
- ⁵E. D. Eastman and W. H. Rodebush, J. Am. Chem. Soc. 40, 489 (1918).
- ⁶T. B. Douglas, A. F. Ball, D. C. Ginnings, and W. D. Davis, J. Am. Chem. Soc. 74, 2472 (1952).

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^o	S° - [G° - H°(T _r)]/T	H° - H°(T _r)	Δ _f H°	
0	0	0	INFINITE	0	0
100	24.631	35.603	89.101	0	0
200	27.004	53.493	67.270	0	0
250	28.008	59.623	63.146	0	0
298.15	29.497	64.670	64.670	0	0
300	29.573	64.833	64.671	0	0
336.350	34.567	68.370	64.880	0	0
350	38.484	69.819	65.044	-2.275	0.094
400	52.287	75.838	66.008	3.940	0.394
				CRYSTAL <--> LIQUID	---
					-0.014
					-0.051

PREVIOUS

CURRENT December 1961

Potassium (K)

K₁(cr)

Potassium (K)

$A_f = 39.0983$ Potassium (K)

LIQUID

Potassium (K)

$S^\circ(298.15 \text{ K}) = [71.403] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$
 $T_{\text{fus}} = 336.35 \text{ K}$

$\Delta_f H^\circ(298.15 \text{ K}) = [2.270] \text{ kJ} \cdot \text{mol}^{-1}$
 $\Delta_{\text{sub}} H^\circ = 2.334 \text{ kJ} \cdot \text{mol}^{-1}$

Enthalpy of Formation

$\Delta_f H^\circ(\text{K}, 1, 298.15 \text{ K})$ is calculated from that of the crystal by adding the enthalpy of fusion and the difference in enthalpy, $H^\circ(336.35 \text{ K}) - H^\circ(298.15 \text{ K})$, between the crystal and liquid.

Heat Capacity and Entropy

The liquid heat capacity values are derived from the enthalpy measurements of Douglas *et al.*¹ The heat capacity curve was extrapolated to 298.15 K and 200 K in a reasonable manner.

The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Vaporization Data

Potassium vaporizes to a mixture of monatomic and diatomic gas. The total vapor pressure reaches 1 atm. at 1037 K. The vapor composition at this temperature is 94.5 mole % monatomic and 5.5 mole % diatomic gas. The enthalpy of vaporization of 39.1 grams of liquid potassium to this equilibrium mixture is 18.38 kcal.

Reference

¹T. B. Douglas, A. F. Ball, D. C. Ginnings, and W. D. Davis, *J. Am. Chem. Soc.* 74, 2472 (1952).

T/K	C_p°	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$		$\log K_f$
		$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	ΔG°	
0						
100						
200						
250						
298.15	32.702	71.403	0.	2.270	0.263	-0.046
300	32.677	71.404	0.060	2.276	0.250	-0.044
336.350	32.139	71.630	1.238	---	---	---
350	31.993	71.799	1.676	0.	0.	0.
400	31.499	80.825	3.263	0.	0.	0.
450	31.067	84.510	4.827	0.	0.	0.
500	30.695	87.763	6.370	0.	0.	0.
600	30.136	93.306	9.410	0.	0.	0.
700	29.824	97.925	12.406	0.	0.	0.
800	29.757	101.901	15.383	0.	0.	0.
900	29.936	105.413	18.363	0.	0.	0.
1000	30.361	108.587	21.378	0.	0.	0.
1039.540	30.604	109.769	22.583	---	---	---
1100	31.031	111.511	24.446	-78.951	4.610	-0.219
1200	31.882	114.247	27.591	-77.884	12.160	-0.529
1300	32.803	116.835	30.825	-76.729	19.617	-0.788
1400	33.723	119.300	34.152	-75.482	26.982	-1.007
1500	34.644	121.658	37.570	-74.143	34.255	-1.193

PREVIOUS:

CURRENT December 1961

Potassium (K)

$K_f(\text{I})$

Potassium (K)

CRYSTAL-LIQUID

0 to 336.35 K crystal
above 336.35 K liquid

Refer to the individual tables for details.

$A_f = 39.0983$ Potassium (K)

$K_1(\text{cr,l})$

T/K	C_p^*	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa		$\log K_f$
		$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0.	INFINITE	-7.082	0.	0.	0.
100	24.631	35.603	-5.350	0.	0.	0.
200	27.004	53.493	-2.755	0.	0.	0.
250	28.008	59.623	-1.381	0.	0.	0.
298.15	29.497	64.670	0.	0.	0.	0.
300	29.573	64.853	0.055	0.	0.	0.
336.3150	34.567	68.370	1.174	1.174	CRYSTAL \leftarrow LIQUID	---
336.3150	32.139	75.310	64.880	3.508	TRANSITION	---
350	31.993	76.586	3.946	0.	0.	0.
400	31.499	80.825	5.533	0.	0.	0.
450	31.067	84.510	7.097	0.	0.	0.
500	30.695	87.763	8.641	0.	0.	0.
600	30.136	93.306	11.680	0.	0.	0.
700	29.824	97.925	14.676	0.	0.	0.
800	29.757	101.901	17.653	0.	0.	0.
900	29.936	105.413	20.636	0.	0.	0.
1000	30.361	108.587	23.648	0.	0.	0.
1039.540	30.604	109.769	24.854	---	FUGACITY = 1 bar	---
1100	31.031	111.511	26.716	-78.951	4.610	-0.219
1200	31.882	114.247	29.862	-77.884	12.160	-0.529
1300	32.803	116.835	33.096	-76.729	19.617	-0.788
1400	33.723	119.300	36.422	-75.482	26.982	-1.007
1500	34.644	121.658	39.840	-74.143	34.255	-1.193

PREVIOUS:

CURRENT December 1961

Potassium (K)

$K_1(\text{cr,l})$

Potassium (K)

IDEAL GAS

Potassium (K)

IP(K, g) = 35009.78 ± 0.02 cm⁻¹
 S^o(298.15 K) = 160.340 ± 0.025 J·K⁻¹·mol⁻¹
 Δ_{sub}H^o(298.15 K) = 89.9 ± 0.4 kJ·mol⁻¹
 Δ_{sub}H^o(298.15 K) = 89.0 ± 0.4 kJ·mol⁻¹

Electronic State	Levels and Quantum Weights	g _e
3s _{1/2}	0	2
3p _{1/2}	12985.170	2
3p _{3/2}	13042.876	4
3s _{1/2}	21026.551	2
3p _{3/2}	34991.2	4
IP	35009.78	

Enthalpy of Formation

The enthalpy of formation of potassium gas, Δ_{sub}H^o(298.15 K) = 89.0 ± 0.4 kJ·mol⁻¹, is chosen to be the value recommended by CODATA.¹ This value was obtained from 2nd and 3rd law treatments of vapor pressure data. The reported vapor pressures were corrected for the effects of K₂(g), using D₀^o = 49.01 kJ·mol⁻¹. At higher pressures an alternate virial treatment was employed.

As stated by CODATA,¹ the selected value is the weighted average of the 3rd law values of Δ_{sub}H^o(298.15 K) calculated from the following studies:

Source	Δ _{sub} H ^o (298.15 K), kJ·mol ⁻¹	Source	Δ _{sub} H ^o (298.15 K), kJ·mol ⁻¹
Haycock and Lamplough ²	89.31 ± 0.65	Venogradov and Volyak ¹³	89.27 ± 0.65
Froock and Rodenbush ³	89.41 ± 0.65	Achener ¹⁴	88.97 ± 0.69
Edmondson and Egerton ⁴	89.71 ± 0.25	Abpil'rain <i>et al.</i> ¹⁵	88.94 ± 0.47
Weiler ⁵	89.71 ± 0.65	Bowles ¹⁶	88.50 ± 1.35
Mayer ⁵	88.58 ± 1.00	Gerasimov <i>et al.</i> ¹⁷	89.43 ± 0.50
Neumann and volker ⁷	89.56 ± 0.25	Sphil'rain and Nikanorov ¹⁸	88.70 ± 0.85
Walling ⁸	88.59 ± 0.75	Schins <i>et al.</i> ¹⁹	88.94 ± 0.50
Makansi <i>et al.</i> ⁹	88.73 ± 0.72	Bonilla ²⁰	88.75 ± 0.65
Buck and Pauly ¹⁰	89.72 ± 0.35	Roeder and Morawitz ²¹	89.59 ± 0.38
Stone <i>et al.</i> ¹¹	88.81 ± 0.90	Kondrat'ev ²²	88.27 ± 0.55
Rigney <i>et al.</i> ¹²	88.90 ± 0.93		

The 2nd law calculations from the above sources led to somewhat more positive values.

Heat Capacity and Entropy

The thermal functions for the five alkali metal monatomic gases are calculated by the same procedure. Observed and estimated atomic energy levels are included in the partition function calculation, using an ionization potential lowering (IP-kT) technique as the cutoff procedure in the energy level summation.²⁴

The lowest lying levels for these metals [14904 cm⁻¹ (Li), 16956 cm⁻¹ (Na), 12578 cm⁻¹ (K), 12578 cm⁻¹ (Cs)] do not contribute to the thermal functions below ~1000 K; there is only a translational contribution below this temperature. Above this approximate temperature, the thermal functions become increasingly sensitive to the partition function cutoff procedure used, due to the combined effect of the observation of atomic energy levels of high principal quantum number and a low ionization potential. Energy levels have been observed up to n = 42 (Li), 59 (Na), 79 (K), 77 (Rb), and 73 (Cs). However, not all predicted levels have been observed for each of these principal quantum numbers. The ionization potentials vary from 43487.29 cm⁻¹ for Li to 31406.1 cm⁻¹ for Cs. In calculating the thermal functions with the inclusion of missing levels up to the high principal quantum numbers just mentioned, the Gibbs energy functions show significant differences (depending on the cutoff procedure) above 3000 K.²⁴

The atomic energy levels have been taken from the compilation of Cortiss and Sugar.¹⁴ Our calculated values for the thermal functions are similar to those recommended by CODATA.¹ They do differ for two reasons, however. First, the entropy differs by 0.1094 J·K⁻¹·mol⁻¹ because this table uses a reference pressure of 1 bar, whereas the CODATA recommendations are based on 1 atm. Second, the entropies at 298.15 K for all alkali metal gases differs by ~0.004 J·K⁻¹·mol⁻¹, presumably due to the use of slightly different values for auxiliary data.

References

- J. D. Cox, chairman, CODATA Task Group on Key Values for Thermodynamics, J. Chem. Thermodyn. 10, 903 (1978).
- C. T. Heycock and F. E. E. Lamplough, Proc. Chem. Soc. 28, 3 (1912).
- F. Froock and W. H. Rodenbush, J. Am. Chem. Soc. 48, 2522 (1926).

Continued on page 1489

K₁(g)

T/K	C _p ^o	S ^o - [C _p ^o (T _o)/T]	H ^o - H ^o (T _o)/T	Δ _{sub} H ^o	Δ _{sub} G ^o	log K _r
0	0	INFINITE	INFINITE	89.885	89.885	INFINITE
100	20.786	137.632	178.820	90.231	90.231	-41.802
200	20.786	152.040	162.241	89.715	70.006	-18.284
250	20.786	156.678	160.682	89.380	65.116	-13.605
298.15	20.786	160.340	160.340	89.000	60.476	-10.595
300	20.786	160.468	160.340	88.984	60.299	-10.499
350	20.786	163.672	160.593	88.152	53.529	-8.506
400	20.786	166.448	161.135	85.584	41.335	-6.464
450	20.786	168.896	161.882	83.060	30.486	-4.866
500	20.786	171.086	162.693	84.555	42.894	-4.881
600	20.786	174.876	164.419	83.594	34.652	-3.017
700	20.786	178.080	166.147	82.677	26.568	-1.983
800	20.786	180.856	167.816	81.778	18.614	-1.215
900	20.786	183.304	169.404	80.875	10.773	-0.625
1000	20.786	185.494	170.993	79.940	3.034	-0.158
1039.540	20.786	186.300	171.476	15.411	---	---
1100	20.786	187.475	172.323	0	0	0
1200	20.787	189.284	173.662	0	0	0
1300	20.789	190.948	174.929	0	0	0
1400	20.793	192.483	176.129	0	0	0
1500	20.801	193.923	177.268	0	0	0
1600	20.814	195.266	178.351	0	0	0
1700	20.836	196.529	179.384	0	0	0
1800	20.868	197.720	180.369	0	0	0
1900	20.914	198.850	181.313	0	0	0
2000	20.975	199.924	182.217	0	0	0
2100	21.056	200.949	183.084	0	0	0
2200	21.157	201.931	183.919	0	0	0
2300	21.281	202.874	184.728	0	0	0
2400	21.431	203.783	185.498	0	0	0
2500	21.606	204.661	186.247	0	0	0
2600	21.809	205.512	186.972	0	0	0
2700	22.043	206.340	187.674	0	0	0
2800	22.307	207.146	188.355	0	0	0
2900	22.605	207.934	189.017	0	0	0
3000	22.936	208.706	189.660	0	0	0
3100	23.306	209.464	190.287	0	0	0
3200	23.714	210.210	190.898	0	0	0
3300	24.123	210.943	191.494	0	0	0
3400	24.589	211.670	192.077	0	0	0
3500	25.107	212.390	192.647	0	0	0
3600	25.666	213.105	193.205	0	0	0
3700	26.270	213.816	193.752	0	0	0
3800	26.920	214.526	194.290	0	0	0
3900	27.618	215.234	194.816	0	0	0
4000	28.345	215.940	195.337	0	0	0
4100	29.124	216.649	195.848	0	0	0
4200	29.962	217.361	196.357	0	0	0
4300	30.848	218.076	196.849	0	0	0
4400	31.145	218.726	197.333	0	0	0
4500	32.003	219.436	197.816	0	0	0
4600	32.892	220.149	198.294	0	0	0
4700	33.767	220.861	198.766	0	0	0
4800	34.664	221.553	199.231	0	0	0
4900	35.385	222.273	199.694	0	0	0
5000	36.319	222.997	200.153	0	0	0
5100	37.263	223.725	200.608	0	0	0
5200	38.212	224.458	201.059	0	0	0
5300	39.163	225.195	201.508	0	0	0
5400	40.111	225.936	201.953	0	0	0
5500	41.052	226.681	202.396	0	0	0
5600	41.980	227.429	202.837	0	0	0
5700	42.977	228.111	203.266	0	0	0
5800	43.337	228.557	203.701	0	0	0
5900	44.172	229.605	204.134	0	0	0
6000	44.978	230.354	204.564	0	0	0

PREVIOUS: June 1962 (1 atm)

CURRENT: December 1983 (1 bar)

Potassium (K)

K₁(g)

IDEAL GAS

Potassium, Ion (K⁺)

IP(K⁺, g) = 255100 ± 100 cm⁻¹
 S^o(298.15 K) = 154.576 ± 0.025 J·K⁻¹·mol⁻¹

Potassium, Ion (K⁺)

K⁺(g)

M_r = 39.09775
 ΔH^o(0 K) = 508.7 ± 0.4 kJ·mol⁻¹
 ΔH^o(298.15 K) = [514.007] kJ·mol⁻¹

Electronic Level and Quantum State	Weight	g
1 ¹ S ₀	0	1

Enthalpy of Formation

ΔH^o(K⁺, g, 0 K) is calculated from ΔH^o(K, g, 0 K) using the spectroscopic value of IP(K) = 35009.78 ± 0.02 cm⁻¹ (418.810 ± 0.000 kJ·mol⁻¹) from Corliss and Sugar.² The ionization limit is converted from cm⁻¹ to kJ·mol⁻¹ using the factor, 1 cm⁻¹ = 0.01196266 kJ·mol⁻¹, which is derived from the 1973 CODATA fundamental constants.³ Rosenstock *et al.*,⁴ and Levin and Lias⁵ have summarized additional ionization and appearance potential data.

ΔH^o(K⁺, g, 298.15 K) is calculated from ΔH^o(K, g, 0 K) by using IP(K) with JANAF¹ enthalpies, H^o(0 K) - H^o(298.15 K), for K(g), K⁺(g), and e⁻(ref). ΔH^o(K → K⁺ + 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 ΔH^o(298.15 K) should be changed by -6.197 kJ·mol⁻¹ if it is to be used in the ion convention that excludes the enthalpy of the electron.

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Corliss and Sugar,² is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function⁶ has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state; the first excited state is approximately 162507 cm⁻¹ above the ground state. Since inclusion of these excited states has no effect on the thermodynamic functions (to 6000 K), we list only the ground state. The reported uncertainty in S^o(298.15 K) is due to uncertainties in the relative ionic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the excited states and use of different fill and cutoff procedures.⁶

References

- ¹JANAF Thermochemical Tables: K(g), [2-31-83]; e⁻(ref), 3-31-82.
- ²C. Corliss and J. Sugar, *J. Phys. Chem. Ref. Data* 8(4), 1109-1145 (1979).
- ³E. R. Cohen and B. N. Taylor, *J. Phys. Chem. Ref. Data* 2, 663 (1973).
- ⁴H. M. Rosenstock, K. Draxl *et al.*, *J. Phys. Chem. Ref. Data* 6, Supp. 1, 783 pp. (1977).
- ⁵R. D. Levin and S. G. Lias, *U. S. Nat. Bur. Stand., NBS-RS-NBS-71*, 634 pp. (1982).
- ⁶J. R. Downey, Jr., The Dow Chemical Company, AFOSR-TR-78-0960, Contract No. F44660-75-1-0048, (1978).

T/K	C _p ^o	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = P ^o = 0.1 MPa		log K _r
		S ^o / J·K ⁻¹ ·mol ⁻¹	-(G ^o - H ^o (T _r))/T	H ^o - H ^o (T _r) / KJ·mol ⁻¹	ΔG ^o / KJ·mol ⁻¹	
0	0	0	INFINITE	-6.197	508.695	
100	20.786	131.869	173.057	-4.119		-84.260
200	20.786	146.277	156.478	-2.040		-83.705
250	20.786	150.915	154.919	-1.001		-70.926
298.15	20.786	154.576	154.576	0	514.007	480.947
300	20.786	154.705	154.577	0.038		480.742
350	20.786	157.909	154.830	1.078		474.245
400	20.786	160.685	155.302	2.117		469.930
450	20.786	163.133	156.119	3.156		464.552
500	20.786	165.323	156.932	4.194		459.116
550	20.786	167.113	158.656	5.232		-39.009
600	20.786	172.317	160.384	6.270		448.083
700	20.786	175.092	162.053	7.308		436.860
800	20.786	177.541	163.641	8.346		425.637
900	20.786	179.731	165.142	9.384		414.414
1000	20.786	181.712	166.560	10.422		403.191
1100	20.786	183.520	167.899	11.460		391.968
1200	20.786	185.184	169.165	12.498		380.745
1300	20.786	186.725	170.365	13.536		369.522
1400	20.786	188.159	171.504	14.574		358.299
1500	20.786	189.500	172.588	15.612		347.076
1600	20.786	190.760	173.620	16.650		335.853
1700	20.786	191.948	174.605	17.688		324.630
1800	20.786	193.072	175.548	18.726		313.407
1900	20.786	194.138	176.451	19.764		302.184
2000	20.786	195.153	177.318	20.802		290.961
2100	20.786	196.120	178.151	21.840		279.738
2200	20.786	197.044	178.952	22.878		268.515
2300	20.786	197.928	179.724	23.916		257.292
2400	20.786	198.777	180.470	24.954		246.069
2500	20.786	199.592	181.190	25.992		234.846
2600	20.786	200.376	181.886	27.030		223.623
2700	20.786	201.132	182.560	28.068		212.400
2800	20.786	201.862	183.213	29.106		201.177
2900	20.786	202.566	183.846	30.144		189.954
3000	20.786	203.248	184.461	31.182		178.731
3100	20.786	203.908	185.059	32.220		167.508
3200	20.786	204.548	185.640	33.258		156.285
3300	20.786	205.168	186.205	34.296		145.062
3400	20.786	205.771	186.755	35.334		133.839
3500	20.786	206.356	187.292	36.372		122.616
3600	20.786	206.926	187.815	37.410		111.393
3700	20.786	207.480	188.325	38.448		100.170
3800	20.786	208.020	188.823	39.486		88.947
3900	20.786	208.546	189.310	40.524		77.724
4000	20.786	209.060	189.785	41.562		66.501
4100	20.786	209.560	190.250	42.600		55.278
4200	20.786	210.050	190.705	43.638		44.055
4300	20.786	210.527	191.150	44.676		32.832
4400	20.786	210.995	191.586	45.714		21.609
4500	20.786	211.451	192.013	46.752		10.386
4600	20.786	211.898	192.431	47.790		-1.837
4700	20.786	212.336	192.841	48.828		-13.064
4800	20.786	212.765	193.243	49.866		-24.291
4900	20.786	213.185	193.638	50.904		-35.518
5000	20.786	213.596	194.025	51.942		-46.745
5100	20.786	214.000	194.406	52.980		-57.972
5200	20.786	214.396	194.779	54.018		-69.199
5300	20.786	214.784	195.146	55.056		-80.426
5400	20.786	215.166	195.506	56.094		-91.653
5500	20.786	215.540	195.861	57.132		-102.880
5600	20.786	215.908	196.209	58.170		-114.107
5700	20.786	216.270	196.552	59.208		-125.334
5800	20.786	216.625	196.889	60.246		-136.561
5900	20.786	216.974	197.221	61.284		-147.788
6000	20.786	217.318	197.548	62.322		-159.015

PREVIOUS: March 1965 (1 atm)

CURRENT: December 1983 (1 bar)

Potassium, Ion (K⁺)

K⁺(g)

IDEAL GAS

Potassium, Ion (K⁺)

EA(K, g) = 0.50147 ± 0.00010 eV
 S°(298.15 K) = 154.577 ± 0.005 J K⁻¹·mol⁻¹

ΔH^o(0 K) = 41.5 ± 1 kJ·mol⁻¹
 ΔH^o(298.15 K) = [34.419] kJ·mol⁻¹

M_r = 39.09885 Potassium, Ion (K⁺)

K⁺(g)

Electronic Level and Quantum State	Weight
ε, cm ⁻¹	g
1S ₀	1
0.0	1

Enthalpy of Formation

The enthalpy of formation, at 0 K, for K⁺(g) is calculated from the adopted electron affinity, EA(K, g) = 0.50147 ± 0.00010 eV (48,384 ± 0.010 kJ·mol⁻¹). This value, recommended by Hotop and Lineberger,⁶ was measured by a tunable laser photodetachment threshold technique.² Additional discussion on K⁺(g) may be obtained in the critical discussions of Hotop and Lineberger,⁶ Rosenstock *et al.*,³ and Massey.⁴

ΔH^o(K⁺, g, 298.15 K) is obtained from ΔH^o(K, g, 0 K) by using EA(K, g) with JANAF³ enthalpies, H^o(0 K) - H^o(298.15 K), for K⁺(g), K(g), and e⁻(ref). ΔH^o(K⁺ → K + 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.*³ ΔH^o(298.15 K) should be changed by +6.197 kJ·mol⁻¹ if it is to be used in the ion convention which excludes the enthalpy of the electron.

Heat Capacity and Entropy

The ground state configuration for K⁺(g) is given by Hotop and Lineberger⁶ and Rosenstock *et al.*³ Lacking any experimental evidence as to the stability of any excited states, we assume that no stable excited states exist.

References

- Hotop and W. C. Lineberger, *J. Phys. Chem. Ref. Data* 4, 539 (1975).
- Slater, F. H. Read, S. E. Novick, and W. C. Lineberger, *Phys. Rev. A* 17, 201 (1978).
- H. M. Rosenstock, K. Draxl *et al.*, *J. Phys. Chem. Ref. Data* 6, Supp. 1, 783 pp. (1977).
- S. W. Massey, "Negative Ions," 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).
- JANAF Thermochemical Tables: K(g), 12-31-83; e⁻(ref), 3-31-82.
- Hotop and W. C. Lineberger, *J. Phys. Chem. Ref. Data*, 14, 731 (1985).

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K _r
	C _p ^o	S° - (G° - H°(T _r))/T	H° - H°(T _r)	ΔG°	
0	0	0	INFINITE	41.501	
100	20.786	131.869	-6.197		-2.430
200	20.786	173.057	-4.119		-1.370
300	20.786	196.478	-2.040		-0.910
400	20.786	207.916	-1.001		-0.672
500	20.786	215.577	0.		-0.556
600	20.786	220.738		13.868	-0.528
700	20.786	224.656		13.740	-0.528
800	20.786	227.317		13.740	-0.528
900	20.786	228.993		13.740	-0.528
1000	20.786	229.932		13.740	-0.528
1100	20.786	230.248		13.740	-0.528
1200	20.786	230.929		13.740	-0.528
1300	20.786	231.869		13.740	-0.528
1400	20.786	233.057		13.740	-0.528
1500	20.786	234.478		13.740	-0.528
1600	20.786	236.119		13.740	-0.528
1700	20.786	237.932		13.740	-0.528
1800	20.786	240.000		13.740	-0.528
1900	20.786	242.317		13.740	-0.528
2000	20.786	244.932		13.740	-0.528
2100	20.786	247.869		13.740	-0.528
2200	20.786	251.119		13.740	-0.528
2300	20.786	254.786		13.740	-0.528
2400	20.786	258.869		13.740	-0.528
2500	20.786	263.369		13.740	-0.528
2600	20.786	268.286		13.740	-0.528
2700	20.786	273.619		13.740	-0.528
2800	20.786	279.369		13.740	-0.528
2900	20.786	285.532		13.740	-0.528
3000	20.786	292.119		13.740	-0.528
3100	20.786	299.132		13.740	-0.528
3200	20.786	306.569		13.740	-0.528
3300	20.786	314.432		13.740	-0.528
3400	20.786	322.719		13.740	-0.528
3500	20.786	331.432		13.740	-0.528
3600	20.786	340.569		13.740	-0.528
3700	20.786	350.132		13.740	-0.528
3800	20.786	360.119		13.740	-0.528
3900	20.786	370.532		13.740	-0.528
4000	20.786	381.369		13.740	-0.528
4100	20.786	392.632		13.740	-0.528
4200	20.786	404.319		13.740	-0.528
4300	20.786	416.432		13.740	-0.528
4400	20.786	429.069		13.740	-0.528
4500	20.786	442.232		13.740	-0.528
4600	20.786	455.919		13.740	-0.528
4700	20.786	470.132		13.740	-0.528
4800	20.786	484.969		13.740	-0.528
4900	20.786	500.432		13.740	-0.528
5000	20.786	516.569		13.740	-0.528
5100	20.786	533.369		13.740	-0.528
5200	20.786	550.832		13.740	-0.528
5300	20.786	568.969		13.740	-0.528
5400	20.786	587.786		13.740	-0.528
5500	20.786	607.286		13.740	-0.528
5600	20.786	627.469		13.740	-0.528
5700	20.786	648.332		13.740	-0.528
5800	20.786	669.869		13.740	-0.528
5900	20.786	692.069		13.740	-0.528
6000	20.786	714.932		13.740	-0.528

PREVIOUS: CURRENT: 1983 (1 bar)

K₂O(g)

Potassium Oxide (KO)

IDEAL GAS

Potassium Oxide (KO)

$S^\circ(298.15\text{ K}) = [238.027 \pm 2.1] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$
 $\Delta H_f^\circ(0\text{ K}) = [72.89 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta H_f^\circ(298.15\text{ K}) = [71.13 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum Weight State	ϵ , cm ⁻¹	g
[11]	0	[4]

$\omega_e = [350] \text{ cm}^{-1}$
 $B_e = [0.3068] \text{ cm}^{-1}$
 $\omega_e x_e = [2.2] \text{ cm}^{-1}$
 $\alpha_e = [0.0027] \text{ cm}^{-1}$
 $\sigma = 1$
 $r_e = [2.2] \text{ \AA}$

Enthalpy of Formation

Brewer and Margrave suggested that the ΔH_f° value for MO(g) from the gaseous ions can be taken as the mean of the corresponding ΔH_f° values for the alkali fluoride and chloride with a maximum uncertainty of 10 kcal·mol⁻¹. We obtain the values $\Delta H_f^\circ(0\text{ K}) = -137.94$ and $-117.7 \text{ kcal}\cdot\text{mol}^{-1}$ for the reactions $\text{K}^+(\text{g}) + \text{F}^-(\text{g}) = \text{KF}(\text{g})$ and $\text{K}^+(\text{g}) + \text{Cl}^-(\text{g}) = \text{KCl}(\text{g})$, respectively. Assuming $\Delta H_f^\circ(0\text{ K}) = -127.83 \text{ kcal}\cdot\text{mol}^{-1}$ for the reaction $\text{K}^+(\text{g}) + \text{O}^-(\text{g}) = \text{KO}(\text{g})$, we calculate $\Delta H_f^\circ(\text{KO}, \text{g}, 298.15\text{ K}) = 19.0 \text{ kcal}\cdot\text{mol}^{-1}$ with the JANAF auxiliary values for the gaseous ions.

Based on the assumption that $D_0^\circ(\text{KO}) = 1/2[D_0^\circ(\text{K}_2) + D_0^\circ(\text{O}_2)]$, or $\Delta H_f^\circ(0\text{ K}) = 64.9 \text{ kcal}\cdot\text{mol}^{-1}$ for the reaction $\text{KO}(\text{g}) = \text{K}(\text{g}) + \text{O}(\text{g})$, we evaluate $\Delta H_f^\circ(\text{KO}, \text{g}, 0\text{ K}) = 15.6 \text{ kcal}\cdot\text{mol}^{-1}$ or $\Delta H_f^\circ(\text{KO}, \text{g}, 298.15\text{ K}) = 15.2 \text{ kcal}\cdot\text{mol}^{-1}$.

According to Somayajulu,² in a sequence of similar diatomic molecules, $k_e r_e D_0^\circ = \text{constant}$, where $k_e = \text{force constant}$ and $r_e = \text{equilibrium bond distance}$. Using $r_e = 1.62 \text{ \AA}$, $D_0^\circ = 77.9 \text{ kcal}\cdot\text{mol}^{-1}$ for LiO(g), $r_e = 2.2 \text{ \AA}$, and $k_e(\text{KO})/k_e(\text{LiO}) = 0.3015$, we calculate $D_0^\circ = 55 \text{ kcal}\cdot\text{mol}^{-1}$ for KO(g), yielding $\Delta H_f^\circ(\text{KO}, \text{g}, 298.15\text{ K}) = 26.1 \text{ kcal}\cdot\text{mol}^{-1}$. The value k_e is derived from the relation $k_e = 4 \cdot \mu^{-2}$, where μ is the vibrational frequency for the diatomic molecule and μ is the reduced mass.

The value of $\Delta H_f^\circ(\text{KO}, \text{g}, 298.15\text{ K})$ is tentatively adopted as $17 \pm 10 \text{ kcal}\cdot\text{mol}^{-1}$.

Heat Capacity and Entropy

The ground state configuration is assumed to be the same as that for the OH(g) molecule, which has the same number of valence electrons. The values of ω_e and $\omega_e x_e$ are estimated by comparison with those for LiF(g) and KF(g). The bond distance is estimated from those for HO(g), HF(g) and KF(g). B_e and α_e are derived from r_e , ω_e and $\omega_e x_e$ by the method suggested by Herzberg.³

References

- ¹L. Brewer and J. Margrave, J. Phys. Chem. 59, 421 (1955).
- ²G. R. Somayajulu, J. Chem. Phys. 33, 1541 (1960).
- ³G. Herzberg, "Spectra of Diatomic Molecules," D. Van Nostrand Co., Inc., New York, (1950).

T/K	C _p ^o	S ^o	J·K ⁻¹ ·mol ⁻¹	-(G ^o -H ^o (T))/RT	H ^o -H ^o (T)/RT	ΔH ^o kJ·mol ⁻¹	Standard State Pressure = p ^o = 0.1 MPa	log K _r
0	0	0	INFINITE	INFINITE	-9.666	72.886	72.886	INFINITE
100	30.583	201.486	268.756	0.6727	-6.727	72.640	64.717	-33.805
200	34.332	223.966	241.275	-3.462	-3.462	71.835	57.109	-14.915
250	35.340	231.744	238.616	-1.718	-1.718	71.496	53.464	-11.171
298.15	35.981	238.027	238.027	0	0	71.128	50.074	-8.764
300	36.001	238.249	238.028	0.067	0.067	71.113	49.893	-8.687
350	36.455	243.835	238.468	1.879	1.879	68.293	46.487	-6.918
400	36.782	248.725	239.451	3.710	3.710	67.792	43.407	-5.668
450	37.029	253.073	240.727	5.555	5.555	67.315	40.387	-4.688
500	37.223	256.984	242.160	7.412	7.412	66.857	37.420	-3.909
600	37.514	263.798	245.215	11.500	11.500	65.976	31.616	-2.752
700	37.731	269.598	248.295	14.912	14.912	65.115	25.957	-1.937
800	37.906	274.648	251.280	18.694	18.694	64.252	20.422	-1.333
900	38.056	279.121	254.130	22.493	22.493	63.365	14.996	-0.870
1000	38.191	283.138	256.833	26.303	26.303	62.433	9.671	-0.505
1100	38.316	286.784	259.393	30.130	30.130	61.515	9.053	-0.430
1200	38.433	290.123	261.816	33.968	33.968	60.610	11.469	-0.499
1300	38.546	293.204	264.114	37.817	37.817	59.722	13.886	-0.558
1400	38.655	296.064	266.295	41.677	41.677	58.855	16.305	-0.608
1500	38.761	298.735	268.370	45.548	45.548	58.007	18.727	-0.652
1600	38.865	301.240	270.347	49.429	49.429	57.160	21.150	-0.690
1700	38.968	303.589	272.234	53.321	53.321	56.325	23.575	-0.724
1800	39.070	305.829	274.039	57.223	57.223	55.503	26.003	-0.755
1900	39.170	307.944	275.768	61.135	61.135	54.694	28.433	-0.782
2000	39.270	309.956	277.428	65.057	65.057	53.906	30.866	-0.806
2100	39.369	311.874	279.023	68.989	68.989	53.132	33.302	-0.828
2200	39.467	313.708	280.558	72.930	72.930	52.374	35.741	-0.849
2300	39.565	315.465	282.038	76.882	76.882	51.633	38.183	-0.869
2400	39.663	317.151	283.466	80.843	80.843	50.909	40.629	-0.884
2500	39.760	318.772	284.846	84.815	84.815	50.200	43.080	-0.900
2600	39.857	320.333	286.181	88.795	88.795	49.506	45.536	-0.915
2700	39.954	321.839	287.474	92.786	92.786	48.825	47.998	-0.929
2800	40.050	323.294	288.727	96.786	96.786	48.157	50.467	-0.941
2900	40.147	324.701	289.944	100.796	100.796	47.502	52.942	-0.954
3000	40.243	326.064	291.125	104.815	104.815	46.859	55.425	-0.965
3100	40.339	327.385	292.274	108.845	108.845	46.238	57.918	-0.976
3200	40.435	328.667	293.391	112.883	112.883	45.638	60.419	-0.986
3300	40.531	329.913	294.479	116.932	116.932	45.059	62.930	-0.996
3400	40.627	331.124	295.539	120.990	120.990	44.499	65.454	-1.006
3500	40.723	332.303	296.573	125.057	125.057	43.957	67.990	-1.015
3600	40.819	333.452	297.581	129.134	129.134	43.434	70.539	-1.024
3700	40.914	334.571	298.566	133.221	133.221	42.927	73.103	-1.032
3800	41.010	335.664	299.528	137.317	137.317	42.435	75.684	-1.040
3900	41.105	336.730	300.468	141.423	141.423	41.956	78.281	-1.048
4000	41.201	337.772	301.388	145.538	145.538	41.491	80.896	-1.056
4100	41.296	338.791	302.288	149.663	149.663	41.040	83.530	-1.064
4200	41.392	339.787	303.169	153.797	153.797	40.602	86.186	-1.072
4300	41.487	340.762	304.032	157.941	157.941	40.177	88.865	-1.079
4400	41.582	341.717	304.877	162.095	162.095	39.765	91.539	-1.087
4500	41.678	342.652	305.706	166.258	166.258	39.366	94.259	-1.094
4600	41.773	343.570	306.519	170.430	170.430	38.980	97.004	-1.102
4700	41.868	344.469	307.317	174.612	174.612	38.607	99.773	-1.109
4800	41.964	345.351	308.101	178.804	178.804	38.246	102.558	-1.116
4900	42.059	346.218	308.870	183.005	183.005	37.896	105.333	-1.123
5000	42.154	347.068	309.625	187.216	187.216	37.557	108.238	-1.131
5100	42.249	347.904	310.368	191.436	191.436	37.229	111.123	-1.138
5200	42.344	348.725	311.097	195.665	195.665	36.912	114.040	-1.146
5300	42.440	349.533	311.815	199.903	199.903	36.605	116.992	-1.153
5400	42.535	350.327	312.521	204.153	204.153	36.308	119.977	-1.161
5500	42.630	351.108	313.215	208.412	208.412	36.021	122.998	-1.168
5600	42.725	351.877	313.899	212.679	212.679	35.744	126.056	-1.176
5700	42.820	352.634	314.572	216.957	216.957	35.477	129.103	-1.183
5800	42.915	353.380	315.234	221.243	221.243	35.220	132.230	-1.191
5900	43.010	354.114	315.887	225.540	225.540	34.972	135.395	-1.199
6000	43.105	354.838	316.530	229.845	229.845	34.733	138.600	-1.207

PREVIOUS: December 1967 (1 atm) CURRENT: December 1967 (1 bar)

K₂O(g)

Potassium Oxide (KO)

K₂O(g)

Potassium Oxide, Ion (KO⁻)

IDEAL GAS

Potassium Oxide, Ion (KO⁻)

T/K	C _p ^o	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = P ^o = 0.1 MPa		log K _r
		S ^o - [C _p ^o - H ^o (T _r)]/T _r	H ^o - H ^o (T _r)/T _r	ΔH ^o	ΔG ^o	
0	0	INFINITE	-9.636	-130.087		
100	30.460	189.920	0.066	-138.126	-149.427	26.179
200	34.190	212.295	1.874	-141.987	-149.498	26.030
250	35.226	220.044	3.702	-143.533	-151.180	22.562
298.15	35.888	226.308	5.545	-145.052	-152.387	19.900
300	35.999	226.530	7.398	-146.552	-153.402	17.806
350	36.379	232.103	11.132	-149.517	-154.230	16.114
400	36.717	236.984	14.922	-152.460	-155.510	13.538
450	36.973	241.324	18.699	-155.460	-156.276	11.661
500	37.173	245.230	22.464	-158.375	-156.621	10.226
600	37.473	252.036	26.272	-161.388	-156.595	9.089
700	37.693	257.830	30.094	-164.418	-156.236	8.161
800	37.870	262.875	33.928	-167.451	-155.962	7.169
900	38.021	267.344	37.775	-170.486	-155.456	6.201
1000	38.155	271.357	41.629	-173.528	-154.762	5.376
1100	38.279	275.000	45.496	-176.577	-153.931	4.662
1200	38.393	278.335	49.373	-179.634	-152.997	4.038
1300	38.506	281.315	53.260	-182.700	-151.984	3.488
1400	38.614	284.271	57.157	-185.777	-150.928	2.998
1500	38.718	286.938	61.064	-188.864	-149.759	2.559
1600	38.820	289.440	64.980	-191.961	-148.497	2.164
1700	38.921	291.797	68.907	-195.068	-147.154	1.804
1800	39.020	294.024	72.843	-198.184	-145.740	1.477
1900	39.118	296.137	76.788	-201.310	-144.265	1.176
2000	39.215	298.145	80.743	-204.455	-142.738	0.900
2100	39.312	300.161	84.708	-207.619	-141.162	0.644
2200	39.408	302.182	88.682	-210.796	-139.548	0.407
2300	39.504	304.206	92.666	-213.989	-137.895	0.187
2400	39.599	306.232	96.659	-217.198	-136.204	0.019
2500	39.694	308.260	100.661	-220.423	-134.474	-0.192
2600	39.788	308.506	104.673	-223.664	-132.706	-0.393
2700	39.883	310.010	108.694	-226.921	-130.900	-0.583
2800	39.977	311.462	112.725	-230.194	-129.064	-0.774
2900	40.071	312.866	116.764	-233.484	-127.200	-0.965
3000	40.165	314.226	120.814	-236.791	-125.312	-1.156
3100	40.258	315.545	124.872	-240.115	-123.400	-1.347
3200	40.352	316.825	128.940	-243.456	-121.464	-1.538
3300	40.445	318.068	133.017	-246.814	-119.504	-1.730
3400	40.538	319.277	137.103	-250.189	-117.520	-1.922
3500	40.632	320.453	141.199	-253.580	-115.512	-2.115
3600	40.725	321.599	145.304	-256.987	-113.480	-2.308
3700	40.818	322.716	149.419	-260.411	-111.424	-2.502
3800	40.911	323.806	153.542	-263.851	-109.344	-2.696
3900	41.004	324.870	157.675	-267.307	-107.240	-2.890
4000	41.097	325.909	161.817	-270.779	-105.112	-3.084
4100	41.190	326.925	165.969	-274.267	-102.960	-3.278
4200	41.283	327.919	170.130	-277.771	-100.784	-3.472
4300	41.376	328.891	174.300	-281.291	-98.592	-3.666
4400	41.468	329.843	178.479	-284.826	-96.384	-3.860
4500	41.561	330.776	182.667	-288.376	-94.160	-4.054
4600	41.654	331.691	186.865	-291.941	-91.920	-4.248
4700	41.747	332.588	191.072	-295.521	-89.664	-4.442
4800	41.839	333.467	195.289	-299.116	-87.392	-4.636
4900	41.932	334.331	199.514	-302.726	-85.104	-4.830
5000	42.025	335.179	203.749	-306.351	-82.792	-5.024
5100	42.117	336.012	207.993	-310.000	-80.464	-5.218
5200	42.210	336.831	212.247	-313.671	-78.120	-5.412
5300	42.302	337.636	216.509	-317.364	-75.760	-5.606
5400	42.395	338.428	220.781	-321.080	-73.384	-5.800
5500	42.488	339.206	225.056	-324.819	-70.992	-6.000
5600	42.580	339.973	229.333	-328.581	-68.584	-6.200
5700	42.673	340.727	233.613	-332.366	-66.160	-6.400
5800	42.765	341.470	237.896	-336.174	-63.720	-6.600
5900	42.858	342.202	242.182	-340.005	-61.264	-6.800
6000	42.950	342.923	246.471	-343.858	-58.792	-7.000

$M_r = 55.09825$ Potassium Oxide, Ion (KO⁻)
 $\Delta H_f^\circ(298.15\text{ K}) = [-130.09 \pm 83.7] \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta H_f^\circ(298.15\text{ K}) = [-138.07 \pm 83.7] \text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum Weight State
 $\epsilon_r, \text{ cm}^{-1}$
 $[\Sigma]$
 0 [1]
 $\omega_e x_e = [2.3] \text{ cm}^{-1}$
 $\alpha_e = [0.0027] \text{ cm}^{-1}$
 $\sigma = 1$
 $r_e = [2.2] \text{ \AA}$

Enthalpy of Formation
 Since the electron affinity of KO(g) is unavailable, the value of $\Delta H_f^\circ(\text{KO}^-, g, 298.15\text{ K})$ is estimated. Assuming that the enthalpy change $\Delta H_f^\circ(0\text{ K})$ of the reaction (1) $\text{KO}(g) = \text{K}(g) + \text{O}^-(g)$ is approximately the average of the $\Delta H_f^\circ(0\text{ K})$ value for the reaction (2) $\text{KO}(g) = \text{K}(g) + \text{O}(g)$ and (3) $\text{KF}(g) = \text{K}(g) + \text{F}(g)$, we obtain $\Delta H_f^\circ(0\text{ K}) = 1/2(63.5 + 117.3) = 90.4 \text{ kcal}\cdot\text{mol}^{-1}$ for reaction (1). However, we compare the $\Delta H_f^\circ(0\text{ K})$ values for the reactions (4) $\text{HO}(g) = \text{H}(g) + \text{O}(g)$, (5) $\text{HO}^-(g) = \text{H}(g) + \text{O}^-(g)$, and (6) $\text{HF}(g) = \text{H}(g) + \text{F}(g)$, and find that $\Delta H_f^\circ(0\text{ K})$ for reaction (5) is experimentally determined as $109.7 \text{ kcal}\cdot\text{mol}^{-1}$, which is about $8 \text{ kcal}\cdot\text{mol}^{-1}$ more negative than the average of $\Delta H_f^\circ(0\text{ K})$ values for reactions (4) and (6). Based on this fact we estimated $\Delta H_f^\circ(0\text{ K}) = 80 \text{ kcal}\cdot\text{mol}^{-1}$ for reaction (1), yielding $\Delta H_f^\circ(\text{KO}^-, g, 298.15\text{ K}) = -33 \text{ kcal}\cdot\text{mol}^{-1}$. The value of $\Delta H_f^\circ(\text{KO}^-, g, 298.15\text{ K})$ is tentatively adopted as $-33 \pm 20 \text{ kcal}\cdot\text{mol}^{-1}$. The electronic affinity of KO(g) is derived to be $2.2 \pm 0.9 \text{ eV}$. The value of EA for HO(g) is determined as $1.8 \pm 0.1 \text{ eV}$.

Heat Capacity and Entropy
 The ground state configuration is assumed to be the same as that of KF(g) which is isolectronic with KO⁻(g). The values of $\omega_e, \omega_e x_e$ and r_e are estimated by comparison with those for KF(g). The values of B_e and α_e are calculated from r_e, ω_e and $\omega_e x_e$ using the method recommended by Herzberg.¹

Reference
 1 G. Herzberg, "Spectra of Diatomic Molecules," D. Van Nostrand Co., Inc. New York, (1950).

CURRENT: December 1967 (1 bar)

PREVIOUS: December 1967 (1 atm)

K₂O(g)

Potassium Oxide, Ion (KO⁻)

K₁O₂(cr)Potassium Superoxide (KO₂)M_r = 71.0971

CRYSTAL

Potassium Superoxide (KO₂)

$S^{\circ}(298.15 \text{ K}) = 122.499 \pm 4.2 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$
 $T_{\text{m}} = 193.5 \text{ K}$
 $T_{\text{m}} = 230.9 \text{ K}$
 $T_{\text{m}} = 782 \pm 20 \text{ K}$

Enthalpy of Formation

D'Orazio and Wood¹ measured the enthalpy of solution, $\Delta_{\text{sol}} H^{\circ}(25^{\circ}\text{C}) = -13.0 \pm 0.4 \text{ kcal mol}^{-1}$ for KO₂(cr) + 1/2 H₂O(l). KOH(aq), 12,000 H₂O + 3/4 O₂(g) which leads to $\Delta_f H^{\circ}(\text{KO}_2, \text{cr}, 298.15 \text{ K}) = -68.09 \pm 0.4 \text{ kcal mol}^{-1}$, using the following auxiliary data, $\Delta_f H^{\circ}(\text{KOH(aq)}, 12,000 \text{ H}_2\text{O}, 298.15 \text{ K}) = -115.243 \text{ kcal mol}^{-1}$, and $\Delta_f H^{\circ}(\text{H}_2\text{O}, \text{l}, 298.15 \text{ K}) = -68.315 \text{ kcal mol}^{-1}$.¹³ Gilles and Margrave⁴ also measured the enthalpy of solution as $-13.2 \pm 0.8 \text{ kcal mol}^{-1}$ from which we obtain $\Delta_f H^{\circ}(\text{KO}_2, \text{cr}, 298.15 \text{ K}) = -67.88 \pm 0.8 \text{ kcal mol}^{-1}$. Both $\Delta_{\text{sol}} H^{\circ}$ values have been corrected for impurities present in their samples. The value $\Delta_f H^{\circ}(\text{KO}_2, \text{cr}, 298.15 \text{ K}) = -68.0 \pm 0.5 \text{ kcal mol}^{-1}$ is adopted in the tabulation.

Kazarnovskaya and Kazarnovskii⁵ and deForcrand⁶ determined the enthalpy of solution in H₂SO₄(aq) and derived the heat of formation of KO₂(cr) as $-67.9 \text{ kcal mol}^{-1}$ and $-66.8 \text{ kcal mol}^{-1}$, respectively. The former is reliable since their sample was well characterized and corrections for the impurities were included in the $\Delta_{\text{sol}} H^{\circ}$ data.⁵ The latter did not give enough experimental details to check their derivation.

Heat Capacity and Entropy

The low temperature heat capacities in the temperature range from 52–298 K are obtained from Todd's measurements.⁷ Two peaks at 193.5 K and 230.9 K were found in his heat capacity data. Below 50 K, the heat capacities were extrapolated using a combination of 1 Debye ($\theta = 139$) and 2 Einstein ($\theta = 260$) functions as suggested by Todd. This extrapolation yields the entropy from lattice contribution as 3.278 cal·K⁻¹·mol⁻¹ at 50 K. By neutron diffraction, Smith *et al.*⁸ found an antiferromagnetic transition at 7 K which indicates the existence of an unpaired electron in KO₂(cr). We tentatively adopt $S^{\circ}(50 \text{ K}) = 4.656 \pm 1 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ which includes both lattice (3.278 cal·K⁻¹·mol⁻¹) and unpaired electron (Rln2) contributions. Heat capacities above 298 K are estimated graphically.

The entropy at 298 K is calculated from the C_p° data and is based on an extrapolation of $S^{\circ}(50 \text{ K}) = 4.656 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$.

Transition Data

Todd⁷ observed two anomalies in the heat capacity at 193.5 and 230.9 K which are adopted as two phase transitions in the tabulation. The heats of transition are calculated from the total heats of absorption given by Todd between 180 and 208 K for transition 1 and 217–240 K for transition 2 with extrapolated C_p° below 176 K and above 250 K.

Smith *et al.*⁸ confirmed these two transitions in the neutron diffraction measurements. In addition, they found an antiferromagnetic transition at 7.1 ± 0.5 K and an unusually low temperature phase transition at 12 K. Neuman⁹ observed a color change at 75.7 ± 15°C in the warming and cooling curves for KO₂(cr). This color change represents a phase transition which is in good agreement with Todd's observation.

Fusion Data

Firsova *et al.*¹⁰ studied the thermograms of KO₂(cr) and found the melting point 509 ± 20°C under atmospheric pressure which is adopted in the tabulation. Earlier melting point data were reported as 380°C by Blumental¹¹ and 440°C by deForcrand.⁶

References

- L. A. D'Orazio and R. H. Wood, *J. Phys. Chem.* **69**, 2550 (1965).
- This value is derived from JANAF $\Delta_f H^{\circ}(\text{KOH}, \text{aq}, \infty, 298.15 \text{ K}) = -115.273 \text{ kcal mol}^{-1}$ with the heat of dilution data from V. B. Parker, *NSRDS-NBS 2*, (1965).
- U. S. Nat. Bur. Stand. Tech. Note 270-3, (1968).
- P. W. Gilles and J. L. Margrave, *J. Phys. Chem.* **60**, 1333 (1956).
- L. I. Kazarnovskaya and I. A. Kazarnovskii, *Zh. Fiz. Khim.* **25**, 293 (1951).
- M. R. deForcrand, *Comp. Rend.* **158**, 843 (1914).
- S. S. Todd, *J. Amer. Chem. Soc.* **75**, 1229 (1953).
- H. G. Smith, R. M. Nicklow, L. J. Raubenheimer and M. K. Wilkinson, *J. Appl. Phys.* **37**, 1047 (1966).
- E. W. Neuman, *J. Chem. Phys.* **3**, 243 (1935).
- T. P. Firsova, A. N. Molodkina, T. G. Morozova and I. V. Aksenova, *Izv. Akad. Nauk SSSR, Ser. Khim. No. 9* (English transl.) 1639 (1965).
- M. Blumental, *Rozmiki Chem.* **12**, 126 (1932); M. Centnerszwer and M. Blumental, *Bull. Intern. Acad. Polonaise, Classe Sci. Math. Nat.* **1933A**, 499.

T/K	Enthalpy Reference Temperature = T, = 298.15 K			Standard State Pressure = P° = 0.1 MPa		
	C _p ^o	S° - [C _p ^o - H ^o (T)]/T	H° - H°(T)	ΔH°	ΔG°	log K _f
0	0	INFINITE	-16.734	-285.480	-285.480	INFINITE
100	52.400	188.849	-14.262	-287.646	-271.377	141.753
200	69.454	129.436	-7.374	-286.263	-255.381	66.699
298.15	77.530	122.499	0	-284.512	-240.589	42.150
300	77.613	122.979	0.144	-284.478	-240.316	41.843
400	83.889	146.226	8.240	-284.851	-225.443	29.440
500	87.653	165.373	16.827	-282.410	-210.868	22.029
600	90.165	181.588	25.724	-279.712	-196.810	17.134
700	91.922	195.625	34.833	-276.854	-183.217	13.672
800	93.220	207.987	44.092	-273.908	-170.041	11.103
900	94.224	219.028	53.467	-270.921	-157.237	9.126
1000	94.893	228.992	62.924	-267.939	-144.765	7.562
1100	95.395	238.061	72.440	-264.951	-132.980	6.077
1200	95.730	246.376	81.997	-262.021	-122.520	4.724
1300	95.981	254.049	91.583	-260.097	-113.388	3.592
1400	96.148	261.169	101.191	-258.182	-105.557	2.633
1500	96.232	267.806	110.810	-256.284	-98.006	1.811

PREVIOUS: June 1962

CURRENT: June 1971

Potassium Superoxide (KO₂)K₁O₂(cr)

Potassium (K₂)

IDEAL GAS

M_r = 78.1966 Potassium (K₂)

K₂(g)

D₀⁰ = 53.48 ± 1.20 kJ·mol⁻¹ (natural abundance)
 S⁰(298.15 K) = 249.690 ± 0.042 J·K⁻¹·mol⁻¹

Δ_fH⁰(0 K) = 127.11 ± 2.0 kJ·mol⁻¹
 Δ_fH⁰(298.15 K) = 123.68 ± 2.0 kJ·mol⁻¹

Spectroscopic Data for ³⁹ K ₂ (Ground State, ¹ Σ _g ⁺) in cm ⁻¹	
ω _e	= 92.021
ω _e x _e	= 0.2829
B _e	= 0.056743
D _e	= 8.63 × 10 ⁻⁴
(a) - 7.2 × 10 ⁻⁶ (ν + 1/2) ² + 1.5 × 10 ⁻⁷ (ν + 1/2) ³	
ω ₃ x ₃	= -2.055 × 10
r _e	= 3.9051 Å

Enthalpy of Formation

Using the adopted value of the dissociation energy for natural abundance K₂(g), D₀⁰ = 53.477 kJ·mol⁻¹ [D₀⁰ = 53.474 kJ·mol⁻¹ as determined by Tango *et al.*¹], and the recommended Δ_fH⁰(K, g, 0 K) = 90.14 kJ·mol⁻¹ from NBS,² we calculate Δ_fH⁰(K₂, g, 0 K) = 126.80 kJ·mol⁻¹. Since this value is only 0.31 kJ·mol⁻¹ smaller than the NBS recommended value of 127.1 kJ·mol⁻¹, we adopt the NBS result. Correcting this value to 298.15 K using the current H⁰(298.15 K) - H⁰(0 K) = 1.0738 kJ·mol⁻¹ for K₂(g) and the NBS value of H⁰(298.15 K) - H⁰(0 K) = 7.092 kJ·mol⁻¹ for K(cr),³ we obtain Δ_fH⁰(K₂, g, 298.15 K) = 123.68 kJ·mol⁻¹.

Heat Capacity and Entropy

The heat capacity and entropy were calculated using a direct summation technique similar to the Li₂(g) species (see Li₂(g) table) using data given above.¹³ Since insufficient spectroscopic data exist for the lower lying excited electronic states, we performed the calculation in the ground state only. Based on the results of Li₂ and Na₂, we expect that the neglect of these excited states results in only ca. 1-2% lower free energy functions near 6000 K. The heat capacity, however, above 2000 K will be seriously deficient. The actual C_v will probably exhibit temperature dependence similar to that calculated for Li₂ and Na₂. Likewise, the actual entropy will be somewhat larger than given here but these effects will not manifest themselves at temperatures less than ca. 3000 K (for Na₂(g) the entropy of the ground state only at 3000 K is only 1.3 J·K⁻¹ less than that calculated including the excited states). Separate calculations were performed on the isotopic species ³⁹K₂, ⁴¹K₂, and ³⁹K³⁹K and the results combined according to the natural atomic isotopic abundances:³ ³⁹K, 93.258%; ⁴¹K, 6.730% (the diatomic species ³⁹K₂ was neglected due to the small isotopic abundance of 0.11%). The spectroscopic input data for the calculation of the isotopic species were calculated from the ³⁹K₂(g) data using mass reduced scaling. The rotational levels were weighted according to the nuclear spins of the individual atoms (³⁹K, I=3/2, ⁴¹K, I=4) as follows: ³⁹K₂, even J weight = 0.625, odd J weight = 0.375, ⁴¹K₂, even J weight = 0.556, odd J weight = 0.444. The adopted value of S⁰(298.15 K) is only 0.15 J·K⁻¹·mol⁻¹ lower than that adopted by NBS.⁴

References

- ¹W. C. Stwalley, Director, Iowa Laser Facility and Professor of Chemistry and Physics, University of Iowa, personal communication, (1982).
- ²W. J. Tango, J. K. Link and R. N. Zare, *J. Chem. Phys.* **49**, 4264 (1968).
- ³Pure Appl. Chem. **47**, 75 (1976).
- ⁴D. D. Wagman, *et al.*, *J. Phys. Chem. Ref. Data* **11**, Supp. 2 (1982).

T/K	C _p ^o	S ^o - [C _p ^o - H ^o (T)]/T	H ^o - H ^o (T)	Δ _f H ^o	Standard State Pressure = P ^o = 0.1 MPa	log K _f
0	0	INFINITE	-10.738	127.110	127.110	INFINITE
100	36.488	208.970	-3.706	126.963	126.963	-59.120
200	37.533	243.115	0	125.488	99.961	-26.107
298.15	37.962	249.690	0	123.683	87.861	-15.382
300	37.969	249.691	0.070	123.644	87.579	-15.249
400	38.347	260.900	3.886	116.504	76.804	-10.030
500	38.698	269.496	7.739	114.141	67.157	-7.016
600	38.895	276.572	11.631	111.944	57.988	-5.047
700	38.769	282.563	15.507	109.838	49.139	-3.607
800	38.242	287.710	19.361	107.738	40.611	-2.632
900	37.158	292.167	23.145	105.536	32.350	-1.878
1000	36.231	296.046	26.824	103.211	24.340	-1.271
1100	34.982	299.441	30.386	-57.265	25.795	-1.225
1200	33.710	302.430	33.820	-57.988	33.377	-1.453
1300	32.482	305.079	37.129	-58.837	41.024	-1.648
1400	31.337	307.444	40.319	-59.805	48.742	-1.819
1500	30.292	309.570	43.400	-60.884	56.532	-1.969
1600	29.352	311.494	46.381	-62.064	64.397	-2.102
1700	28.514	313.248	49.274	-63.336	72.339	-2.223
1800	27.771	314.856	52.087	-64.693	80.356	-2.332
1900	27.114	316.340	54.831	-66.127	88.456	-2.430
2000	26.533	317.716	57.512	-67.634	96.631	-2.524
2100	26.020	318.998	60.140	-69.209	104.883	-2.609
2200	25.566	320.197	62.718	-70.851	113.211	-2.688
2300	25.162	321.325	65.254	-72.559	121.616	-2.762
2400	24.804	322.388	67.752	-74.332	130.096	-2.831
2500	24.485	323.394	70.217	-76.171	138.651	-2.897
2600	24.248	324.348	72.651	-78.078	147.282	-2.959
2700	23.944	325.257	75.057	-80.055	155.986	-3.018
2800	23.715	326.124	77.440	-82.107	164.776	-3.074
2900	23.508	326.952	79.801	-84.237	173.621	-3.127
3000	23.321	327.746	82.143	-86.449	182.549	-3.178
3100	23.153	328.508	84.466	-88.749	191.553	-3.228
3200	23.009	329.240	86.774	-91.142	200.653	-3.275
3300	22.886	329.946	89.066	-93.617	209.788	-3.321
3400	22.783	330.626	91.346	-96.209	219.021	-3.368
3500	22.617	331.284	93.613	-98.907	228.351	-3.408
3600	22.510	331.919	95.870	-101.727	237.720	-3.449
3700	22.412	332.535	98.116	-104.674	247.189	-3.490
3800	22.322	333.131	100.352	-107.755	256.740	-3.529
3900	22.240	333.710	102.580	-110.980	266.375	-3.568
4000	22.163	334.272	104.801	-114.344	276.091	-3.605
4100	22.092	334.818	107.013	-117.870	285.896	-3.642
4200	22.026	335.350	109.219	-121.572	295.788	-3.679
4300	21.966	335.868	111.419	-125.452	305.769	-3.714
4400	21.909	336.372	113.612	-129.509	315.791	-3.749
4500	21.856	336.864	115.801	-133.091	325.944	-3.783
4600	21.807	337.343	117.984	-137.397	336.192	-3.818
4700	21.761	337.812	120.162	-141.847	346.532	-3.854
4800	21.718	338.270	122.336	-146.267	356.944	-3.881
4900	21.677	338.717	124.506	-151.081	367.477	-3.917
5000	21.640	339.155	126.672	-156.086	378.110	-3.950
5100	21.604	339.583	128.834	-161.281	388.847	-3.983
5200	21.571	340.002	131.093	-166.670	399.684	-4.015
5300	21.539	340.412	133.148	-172.252	410.629	-4.047
5400	21.510	340.815	135.200	-178.027	421.681	-4.079
5500	21.482	341.209	137.450	-183.994	432.841	-4.111
5600	21.456	341.596	139.977	-190.151	444.111	-4.142
5700	21.431	341.976	141.741	-196.505	455.399	-4.173
5800	21.407	342.348	143.883	-202.245	466.878	-4.205
5900	21.385	342.714	146.025	-208.356	478.472	-4.236
6000	21.364	343.073	148.160	-215.654	490.178	-4.267

PREVIOUS: June, 1962 (1 atm)

CURRENT: December, 1983 (1 bar)

Potassium (K₂)

K₂(g)

K₂O₁(cr)Potassium Oxide (K₂O)M_r = 94.1960

CRYSTAL

Potassium Oxide (K₂O)

S°(298.15 K) = [94.14 ± 6.3] J·K⁻¹·mol⁻¹
 $\Delta_f H^\circ(0 \text{ K}) = \text{Unknown}$
 $\Delta_f H^\circ(298.15 \text{ K}) = -363.17 \pm 2.1 \text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation

$\Delta_f H^\circ(298.15 \text{ K})$ was reported by Rengade¹ based on the measurements of the enthalpy of solution of K(cr) and K₂O(cr) in H₂O. The same value of $\Delta_f H^\circ(298.15 \text{ K})$ was also given by de Forcrand.²

Heat Capacity and Entropy

Both C_p° and S°(298.15 K) were estimated by comparison with those of the Na₂O(cr).

Decomposition Data

T_{dec} = 1154 K(600mmHg) was taken from NRC Bulletin.³

References

- ¹M. Rengade, Ann. Chim. et phys. (8) 14, 540 (1908).
- ²R. de Forcrand, Compt. rend. 158, 991 (1914).
- ³Data on Chemicals for Ceramic Use, National Research Council Bulletin 118 (1949).

T/K	C _p ^o	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K _r
		S°	-[G° - H°(T _r)]/T	H° - H°(T _r)	Δ _r H°	
		J·K ⁻¹ ·mol ⁻¹	J·K ⁻¹ ·mol ⁻¹	KJ·mol ⁻¹	KJ·mol ⁻¹	
0						
100						
200						
250						
298.15	83.680	94.140	94.140	0.	-363.171	56.429
300	83.889	94.658	94.142	0.155	-363.153	56.037
400	91.546	119.958	97.539	8.968	-366.782	40.133
500	94.266	140.671	104.161	18.255	-365.240	30.572
600	97.404	158.126	111.736	27.834	-363.320	24.277
700	101.384	173.439	119.478	37.773	-361.000	19.722
800	105.395	187.239	127.099	48.111	-358.283	16.367
900	109.455	199.867	134.494	58.854	-355.209	13.778
1000	113.512	211.629	141.627	70.002	-351.817	11.726
1100	117.549	222.637	148.496	81.555	-306.056	9.626
1200	121.592	233.038	155.112	93.512	-500.031	7.635
1300	125.642	242.931	161.489	105.874	-493.618	5.971
1400	129.699	252.390	167.647	118.641	-486.816	4.563
1500	133.762	261.477	173.601	131.814	-479.623	3.361
1600	137.833	270.240	179.369	145.394	-472.038	2.325
1700	141.910	278.718	184.965	159.381	-464.062	1.426
1800	145.993	286.945	190.403	173.776	-455.695	0.641
1900	150.083	294.948	195.696	188.580	-446.939	-0.049
2000	154.180	302.751	200.854	203.793	-437.796	-0.657

PREVIOUS

CURRENT: June 1963

Potassium Oxide (K₂O)K₂O₁(cr)

$K_2O_2(cr)$

$M_r = 110.1954$ Potassium Peroxide (K_2O_2)

CRYSTAL

Potassium Peroxide (K_2O_2)

$S^\circ(298.15\text{ K}) = [112.968 \pm 6.3] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ $\Delta_f H^\circ(0\text{ K}) = \text{Unknown}$
 $T_{\text{fus}} = 763\text{ K}$ $\Delta_f H^\circ(298.15\text{ K}) = [495.80 \pm 4.2] \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{sub}} H^\circ = \text{Unknown}$

Enthalpy of Formation

$\Delta_f H^\circ(298.15\text{ K})$ was reported by NBS.¹ The value was based on the measured decomposition pressure of $K_2O_2(cr)$ by Centnerzwer and Blumenthal.²

Heat Capacity and Entropy

The heat capacities and $S^\circ(298.15\text{ K})$ were estimated by comparison with those for $Na_2O_2(cr)$, $Na_2O(cr)$, and $K_2O(cr)$.

Fusion Data

T_{fus} was reported by Centnerzwer and Blumenthal.²

References

- ¹D. D. Wagman, U. S. Nat. Bur. Stand., Report 7437, Table 4, Chap. B4, p 95, (January 1, 1962).
- ²M. Centnerzwer and M. Blumenthal, IX Congr. IUPAC, 3A, 201 (1935).

T/K	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$	
	C_p°	$S^\circ - [G^\circ - F^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f G^\circ$
0				
100				
200				
250				
298.15	100.165	112.968	0.	-495.804
300	100.374	113.588	0.185	-429.758
400	107.110	143.348	10.546	-429.348
500	115.478	168.206	21.702	-406.479
600	120.708	189.704	33.501	-383.461
700	127.952	208.862	45.938	-360.801
800	134.725	226.395	59.076	-348.798
900	140.798	242.614	72.852	-337.206
1000	146.858	257.762	87.235	-296.134
1100	152.917	272.043	102.274	-275.378
1200	158.959	285.608	117.818	-246.314
1300	164.983	298.569	134.015	-211.675
1400	170.992	311.016	150.814	-177.717
1500	176.983	323.018	168.213	-144.431
1600	182.958	334.631	186.210	-111.812
1700	188.916	345.901	204.804	-79.850
1800	194.857	356.868	223.993	-48.542
1900	200.782	367.562	243.775	-17.883
2000	206.690	378.011	264.148	0.519
				-0.334
				-1.084

PREVIOUS: June 1963

CURRENT: September 1963

Potassium Peroxide (K_2O_2)

$K_2O_2(cr)$

K₂O₃Si₁(cr)Potassium Silicate (K₂SiO₃)M_r = 154.2803

CRYSTAL

Potassium Silicate (K₂SiO₃)

T/K	C _p ^a	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _f
		S ^b - [G° - H°(T _r)]/T	H° - H°(T _r)	ΔH°	ΔG°	
0	0	INFINITE	-21.870	-1539.542	-1539.542	INFINITE
100	63.262	46.944	-18.949	-1544.710	-1515.904	791.877
200	98.198	103.052	-10.657	-1547.151	-1485.986	388.100
298.15	118.407	146.147	0	-1548.080	-1455.733	255.038
300	118.758	146.881	0.219	-1548.089	-1455.160	253.366
400	135.562	183.448	12.971	-1552.872	-1423.255	185.858
500	148.114	215.101	27.179	-1551.745	-1390.957	145.312
600	157.737	242.994	42.492	-1549.626	-1358.985	118.310
700	164.850	267.859	58.632	-1546.808	-1327.426	99.054
800	170.707	290.268	75.420	-1543.488	-1296.307	84.640
900	175.310	310.648	92.728	-1539.816	-1265.627	73.455
1000	179.075	329.321	110.455	-1535.919	-1235.369	64.529
1100	182.004	346.523	128.505	-1531.825	-1196.287	56.807
1200	185.351	362.515	146.887	-1527.596	-1151.692	50.132
1249.000	186.376	369.955	155.996	-1523.256	-1107.622	44.505
1300	187.443	377.434	165.526	-1518.768	-1064.047	39.700
1400	189.535	391.401	184.375	-1504.549	-1020.940	35.552
1500	191.627	404.549	203.434	-1490.983	-978.278	31.937
1600	193.719	416.983	222.701	-1477.077	-935.594	28.747
1700	195.811	428.790	242.177	-1463.823	-892.750	25.850
1800	197.903	440.042	261.865	-1451.228	-850.795	23.269
1900	199.995	450.798	281.758	-1439.292	-809.779	20.957
2000	202.087	461.110	301.879	-1428.016	-769.750	18.874
2100	204.179	471.020	322.175	-1417.400	-730.780	16.989
2200	206.271	480.567	342.698	-1407.452	-692.928	15.331

S°(298.15 K) = 146.147 ± 0.8 J·K⁻¹·mol⁻¹
 T_{fus} = 1249 K
 $\Delta_f H^\circ(10\text{ K}) = -1539.54 \pm 8.4\text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_f H^\circ(298.15\text{ K}) = -1548.08 \pm 8.4\text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{ref}} H^\circ = [50\ 208 \pm 12.6]\text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation

Hatton *et al.*¹ conducted enthalpy of solution measurements on K₂SiO₃(cr) and KOH(cr) in HF(aq) to determine the enthalpy of formation of the silicate. The results of this work gave a $\Delta_f H^\circ(298.15\text{ K}) = -17.5 \pm 0.5\text{ kcal mol}^{-1}$ for the process 2 KOH(cr) + SiO₂(cr, quartz) → K₂SiO₃(cr) + H₂O(l). When combined with the auxiliary data for H₂O(l) KOH(cr) and SiO₂(cr),^{2,3} we calculate $\Delta_f H^\circ(\text{K}_2\text{SiO}_3, \text{cr}, 298.15\text{ K}) = -369.9 \pm 1\text{ kcal}\cdot\text{mol}^{-1}$.

Urusov⁴ summarized the various methods of estimating the enthalpies of formation of silicates using the Born Haber cycle and energies of atomization. His estimate for $\Delta_f H^\circ(\text{K}_2\text{SiO}_3, \text{cr}, 298.15\text{ K})$ is $-369\text{ kcal}\cdot\text{mol}^{-1}$.

An earlier estimate by Wilcox and Bromley⁵ based upon ionic contributions to crystal lattice energies gave $\Delta_f H^\circ(\text{K}_2\text{SiO}_3, \text{cr}, 298.15\text{ K}) = -367 \pm 15\text{ kcal}\cdot\text{mol}^{-1}$.

An attempt to calculate the $\Delta_f H^\circ(\text{K}_2\text{SiO}_3, \text{cr}, 298.15\text{ K})$ from HF solution experiments on higher potassium silicates (K₂S₂O₇, K₂Si₂O₇) and sodium silicates⁶ yielded a value of $-383.8\text{ kcal}\cdot\text{mol}^{-1}$, which is discrepant with the former values.

A value for $\Delta_f H^\circ(\text{K}_2\text{SiO}_3, \text{cr}, 298.15\text{ K}) = -370 \pm 2\text{ kcal}\cdot\text{mol}^{-1}$ has been selected.

Heat Capacity and Entropy

The low temperature heat capacity of K₂SiO₃(cr) has been measured and reported by Stull *et al.*⁷ in the range 15–298 K. They report S°(298.15 K) = 34.93 cal·K⁻¹·mol⁻¹, which is derived from C_p° and an extrapolation of S°(15 K) = 0.18 cal·K⁻¹·mol⁻¹.

Heat capacities above 298.15 K have been estimated by analogy with other alkali metal silicates and borates.

Fusion Data

A melting temperature of 1249 K for K₂SiO₃ was measured by Morey and Bowen.⁸ The enthalpy of fusion, $\Delta_{\text{fus}} H^\circ = 12 \pm 3\text{ kcal}\cdot\text{mol}^{-1}$, was estimated by comparison with other silicates.

References

- W. E. Hatton, D. L. Hildenbrand, G. C. Sinke and D. R. Stull, unpublished data, The Dow Chemical Company, Midland, MI (1959).
- U. S. Nat. Bur. Stand. Tech. Note 270-3, (1968).
- JANAF Thermochemical Tables KOH(cr), 12-31-70; SiO₂(cr), 6-30-67.
- V. S. Urusov, Geokhimiya, No. 5, 551 (1965).
- D. E. Wilcox and L. A. Bromley, Ind. Eng. Chem. 55, No. 7, 32 (1963).
- G. W. Morey, Geophysical Laboratory, Carnegie Institute of Washington, Paper No. 1215 (1952-1953).
- D. R. Stull, D. L. Hildenbrand, F. L. Oetting and G. C. Sinke, J. Chem. Eng. Data 15, 15 (1970).
- G. W. Morey and H. L. Bowen, J. Phys. Chem. 28, 1167 (1924).

PREVIOUS:

CURRENT: June 1972

Potassium Silicate (K₂SiO₃)K₂O₃Si₁(cr)

Potassium Silicate (K₂SiO₃)

M_r = 154.2803 Potassium Silicate (K₂SiO₃)

LIQUID

K₂O₃Si₁(l)

S°(298.15 K) = [184.256] J·K⁻¹·mol⁻¹
T_m = 1249 K

Δ_{cr}H°(298.15 K) = [-1499.290] kJ·mol⁻¹
Δ_{cr}H°[50.208 ± 12.6] kJ·mol⁻¹

Enthalpy of Formation

Δ_{cr}H°(K₂SiO₃, l, 298.15 K) is calculated from that of the crystal by adding the enthalpy of fusion, Δ_mH°, and the difference in enthalpy, H°(1249 K) - H°(298.15 K), between the crystal and liquid.

Heat Capacity and Entropy

The heat capacity of K₂SiO₃(l) has been estimated. A constant C_p° of 43 cal·K⁻¹·mol⁻¹ for K₂SiO₃(l) was selected above a hypothetical glass transition temperature of 700 K. Below this temperature the heat capacity was taken as that of the crystal S°(K₂SiO₃, 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.

T/K	C _p °	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _f
		S° - [C _p ° - H°(T _r)]/T _r	H° - H°(T _r)	Δ _{cr} H°	Δ _{cr} G°	
0			0.			
100						
200						
298.15	118.407	184.256	184.256	-1499.291	-1418.306	248.481
300	118.758	184.990	184.259	-1499.299	-1417.803	246.861
400	135.562	221.557	189.130	-1504.082	-1389.709	181.477
500	148.114	253.210	198.852	-1507.956	-1361.222	142.200
600	157.737	281.103	210.282	-1500.837	-1333.061	116.053
700	164.850	305.985	222.209	-1498.008	-1305.314	97.404
700.000	164.850	305.985	222.209			
700.000	179.912	305.985	222.209			
800	179.912	330.008	234.216	-1493.485	-1278.097	83.451
900	179.912	351.199	246.060	-1489.129	-1251.437	72.632
1000	179.912	370.155	257.538	-1484.968	-1225.251	64.001
1100	179.912	387.302	268.568	-1480.934	-1190.252	56.520
1200	179.912	402.956	279.124	-1478.999	-1149.720	50.086
1249.000	179.912	410.154	284.121	-1478.000	-1109.670	44.587
1300	179.912	417.357	289.211	-1477.043	-1070.056	39.974
1400	179.912	430.690	298.846	-1475.173	-1030.842	35.897
1500	179.912	443.103	308.055	-1474.367	-991.994	32.385
1600	179.912	454.714	316.862	-1473.610	-953.040	29.283
1700	179.912	465.621	325.295	-1472.900	-914.875	26.462
1800	179.912	475.905	333.379	-1472.234	-877.106	23.946
1900	179.912	485.632	341.139	-1471.610	-840.445	21.689
2000	179.912	494.860	348.596	-1471.028	-805.445	19.654
2100	179.912	503.638	355.772	-1470.485	-771.810	17.810
2200	179.912	512.008	362.685	-1470.000	-739.296	16.131
2300	179.912	520.005	369.352	-1469.570	-707.821	14.598
2400	179.912	527.662	375.790	-1469.190	-677.303	13.192
2500	179.912	535.006	382.013	-1468.860	-647.750	11.898
2600	179.912	542.063	388.034	-1468.580	-619.169	10.703
2700	179.912	548.853	393.865	-1468.350	-591.557	9.598
2800	179.912	555.396	399.518	-1468.170	-564.914	8.571
2900	179.912	561.709	405.002	-1468.040	-539.245	7.616
3000	179.912	567.808	410.328	-1467.960	-514.558	

PREVIOUS:

CURRENT: June 1972

Potassium Silicate (K₂SiO₃)

K₂O₃Si₁(l)

0 to 1249 K crystal
above 1249 K liquid

Refer to the individual tables for details.

T/K	C _p ^o	S ^o - J ^o - K ^o · mol ⁻¹	H ^o - H ^o (T ₁)/T	Standard State Pressure = p ^o = 0.1 MPa kJ · mol ⁻¹	log K _r
0	0	0	INFINITE	-1539.542	INFINITE
100	63.262	46.944	236.438	-1515.904	791.827
200	98.198	103.052	156.335	-1547.151	388.100
298.15	118.407	146.147	146.147	-1485.986	255.038
300	118.758	146.881	146.149	-1455.733	253.366
400	135.562	183.448	151.021	-1452.872	183.858
500	148.114	215.101	160.743	-1551.745	148.312
600	157.737	242.984	172.173	-1358.985	118.310
700	164.850	267.859	184.099	-1327.426	99.054
800	170.707	290.268	195.997	-1296.507	84.640
900	175.310	310.648	207.617	-1265.627	73.455
1000	179.075	329.321	218.867	-1235.369	64.529
1100	182.004	346.523	229.700	-1196.287	56.807
1200	185.351	362.515	240.110	-1151.692	50.132
1249.000	186.376	369.955	245.059	CRYSTAL <- -> LIQUID TRANSITION	
1300	179.912	417.354	251.677	-1627.403	44.587
1400	179.912	430.687	263.994	-1621.773	39.924
1500	179.912	443.099	275.525	-1616.227	35.897
1600	179.912	454.711	286.365	-1610.764	32.385
1700	179.912	465.618	296.592	-1605.560	29.283
1800	179.912	475.901	306.271	-1600.032	26.462
1900	179.912	485.629	315.457	-1644.548	23.946
2000	179.912	494.857	324.198	-1639.109	21.689
2100	179.912	503.635	332.535	-1633.718	19.654
2200	179.912	512.004	340.504	-1628.380	17.809
2300	179.912	520.002	348.136	-1623.098	16.131
2400	179.912	527.659	355.458	-1617.876	14.598
2500	179.912	535.003	362.494	-1612.720	13.191
2600	179.912	542.059	369.265	-1607.634	11.897
2700	179.912	548.849	375.791	-1602.623	10.703
2800	179.912	555.392	382.098	-1597.692	9.597
2900	179.912	561.706	388.175	-1592.847	8.571
3000	179.912	567.805	394.062	-1588.095	7.616

PREVIOUS:

CURRENT, June 1972

K₂O₃S₁(cr)

Potassium Sulfate, Alpha (K₂SO₄)

CRYSTAL(α)

Potassium Sulfate (α-K₂SO₄)

M_r = 174.2542

T/K	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
	C _p ^o	S° - (G° - H°(T _r))/T _r	H° - H°(T _r)	Δ _f H°	
0	0	0	INFINITE	-1427.199	INFINITE
100	79.195	61.609	277.387	-1433.305	729.421
200	110.667	127.344	186.920	-1436.245	354.737
298.15	131.319	175.544	175.544	-1437.706	231.188
300	131.666	176.357	175.546	-1437.723	229.634
400	147.649	216.494	180.911	-1445.229	166.909
500	160.733	250.870	191.544	-1446.060	129.153
600	172.527	281.186	204.005	-1445.597	103.978
700	186.368	308.829	217.031	-1442.295	86.012
800	199.619	334.580	230.132	-1439.833	72.564
857.000	207.169	348.575	237.547	95.151	--- ALPHA <--- BETA
900	212.865	358.856	243.098	104.182	62.072
1000	226.116	381.969	255.838	126.131	53.454
1100	239.365	404.142	268.319	149.405	46.001
1200	252.613	425.538	280.534	174.004	39.570

$\Delta_f H^\circ(0\text{ K}) = -1427.20 \pm 0.4\text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_f H^\circ(298.15\text{ K}) = -1437.71 \pm 0.4\text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{tr}} H^\circ(\alpha \rightarrow \beta) = 8.452 \pm 0.418\text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation
 Shibata *et al.*¹ measured the emf of the cell K (amalgam, 0.22019% K₂SO₄(sat. soln.), Hg₂SO₄/Hg at 298 K. From their results at 298 K, correcting the observed voltage for the formation of the K-amalgam, and converting to absolute volts, we have E_{cell} = 3.59172 volts for the reaction at 298 K, 2 K(cr) + Hg₂SO₄(cr) = 2 Hg(l) + K₂SO₄(cr). From this voltage, we calculate Δ_fG°(298.15 K) = -165.656 kcal mol⁻¹. Taking Δ_fG°(Hg₂SO₄, cr, 298.15 K) = -149.658 kcal mol⁻¹ and reference entropies from², we calculate Δ_fG°(K₂SO₄, cr, 298.15 K) = -315.314 kcal mol⁻¹ and Δ_fH°(K₂SO₄, cr, 298.15 K) = -343.525 ± 0.2 kcal mol⁻¹.

The enthalpy of solution at infinite dilution, Δ_{sol}H°(K₂SO₄, cr, 298.15 K) = 5.677 ± 0.020 kcal mol⁻¹, adopted in this tabulation is based on our reanalysis of the enthalpy of solution measurements of Mishchenko and Pronina,³ Tsvetkov and Rabinovich,⁴ Romanova and Samoilov,⁵ Cohen and Kooy,⁶ Bronsted,⁷ Samoilov *et al.*⁸ and Gritsus *et al.*⁹ Enthalpies of dilution are taken from Lange and Streeck.¹¹ When this result is combined with enthalpy of formation of the infinitely dilute ions from CODATA,² we obtain Δ_fH°(K₂SO₄, aq, ∞, 298.15 K) = -337.940 ± 0.10 kcal mol⁻¹ and Δ_fH°(K₂SO₄, cr, 298.15 K) = -343.617 ± 0.10 kcal mol⁻¹.

The solubility of K₂SO₄(cr) in water at 298 K has been measured by many workers.^{4,12,14-16} When the solubility of 0.6919 molal is combined with the activity coefficient data of Stokes,¹³ we obtain Δ_fG°(298.15 K) = 2423 ± 20 cal mol⁻¹ for the reaction K₂SO₄(cr) = 2 K⁺(aq, ∞) + SO₄²⁻(aq, ∞). When this result is combined with enthalpies of formation and entropies from³ we obtain Δ_fH°(K₂SO₄, cr, 298.15 K) = 343.595 ± 0.2 kcal mol⁻¹.

We adopt the value of Δ_fH°(298.15 K) obtained from the enthalpy of solution measurements.

Heat Capacity and Entropy
 Low temperature heat capacities of K₂SO₄(cr, α) have been measured by Moore and Kelley¹⁷ from 52.7-295.4 K and by Paukov¹⁸ from 12.5-299.5 K. The heat capacities reported by Moore and Kelley are systematically lower by about 0.5% than those of Paukov. Our adopted value of S°(298.15 K) = 41.956 ± 0.2 cal K⁻¹ mol⁻¹ is based on S°(12.5 K) = 0.068 cal K⁻¹ mol⁻¹ and H°(12.5 K) - H°(0 K) = 0.640 cal K⁻¹ mol⁻¹ derived from a Debye T³ law extrapolation.

Heat capacity data measured by adiabatic calorimetry in the range 298.5-773.7 K have been reported by Shmidt.¹⁹ In addition, drop calorimetric measurements have been reported by the following workers: Shomate and Naylor,²⁰ Dworkin and Bredig,²¹ Demelou *et al.*²² and Rubinchik *et al.*²³ The heat capacity and enthalpy curves between 298 K and 857 K are obtained by orthogonal polynomial curve fitting of all the data listed above. These data are in good agreement.

Transition Data
 K₂SO₄(cr, α) is the low temperature form (sometimes denoted as K₂SO₄, II). The mineral is known as arcanite and exists in the form of orthorhombic crystals (space group D_{2h}²⁶ - Pnma).²⁴ The orthorhombic-to-hexagonal transition temperature for K₂SO₄ is selected as 857 ± 1 K from the calorimetric work of Dworkin and Bredig²¹ and Rubinchik *et al.*²³ and the polymorphism study of Pistorius and Rapoport.²⁵ The enthalpy of transition is determined by taking the difference between the adopted enthalpy curves of α and β-K₂SO₄ extrapolated to 857 K.

References
¹F. L. E. Shibata, S. Oda, and S. Furukawa, *J. Sci. Hiroshima Univ. (Japan)* **3A**, 227 (1933).
²JANAF CODATA Task Group on Key Values for Thermodynamics, *J. Chem. Thermodyn.* **10**, 903 (1978).
³JANAF Thermochemical Tables: K(ref. st.), 12.31 61; O₂(ref. st.), 3-31-77; S(ref. st.), 9-30-77; K₂SO₄(cr, β), 9-30-78.
⁴K. P. Mishchenko and M. S. Pronina, *J. Gen. Chem.* **6**, 85 (1936).
⁵V. G. Tsvetkov and I. B. Rabinovich, *Russ. J. Phys. Chem.* **43**, 675 (1969).
⁶I. I. Romanova and O. Ya. Samoilov, *Russ. J. Inorg. Chem.* **14**, 131 (1969).
⁷E. Cohen and J. Kooy, *Z. Phys. Chem.* **139**, 273 (1928).
⁸J. N. Bronsted, *Z. Phys. Chem.* **77**, 315 (1911).
⁹O. Ya. Samoilov, H. K' O yuan, and T. A. Nosova, *J. Struct. Chem.* **1**, 379 (1960).
¹⁰B. V. Gritsus, E. I. Akhumov, and L. P. Zhilina, *J. Appl. Chem. USSR* **45**, 1969 (1972).
¹¹E. Lange and H. Streeck, *Z. Phys. Chem.* **152**, 1 (1931).
¹²T. Ishii and S. Fujita, *J. Chem. Eng. Data* **23**, 19 (1978).
¹³R. H. Stokes, *Trans. Faraday Soc.* **44**, 295 (1948).
¹⁴S. Z. Makarov and I. G. Druzhinin, *Izv. Akad. Nauk SSSR, Ser. Khim.* 1291 (1937).
¹⁵A. P. Perova, *Zh. Prikl. Khim.* **11**, 1045 (1930).
¹⁶J. N. Pearce and H. C. Eckstrom, *J. Amer. Chem. Soc.* **59**, 2689 (1937).
¹⁷G. E. Moore and K. K. Kelley, *J. Amer. Chem. Soc.* **64**, 2949 (1942).
¹⁸I. E. Paukov, *Russ. J. Phys. Chem.* **43**, 1134 (1969).
¹⁹N. E. Shmidt, *Russ. J. Inorg. Chem.* **12**, 929 (1967).

Continued on page 1489

Potassium Sulfate, Alpha (K₂SO₄)

K₂O₃S₁(cr)

PREVIOUS: December 1971 CURRENT: June 1978

Potassium Sulfate (K₂SO₄) LIQUID

M_f = 174.2542 Potassium Sulfate (K₂SO₄)

K₂O₃S₁(l)

S°(298.15 K) = [211.505] J·K⁻¹·mol⁻¹
 T_{inf}(β → l) = 1342 ± 1 K
 T_{dem} = 2567 K
 $\Delta H_f^\circ(298.15 \text{ K}) = [-1393.668] \text{ kJ}\cdot\text{mol}^{-1}$
 $\Delta_{\text{dem}}H^\circ(\beta \rightarrow \text{l}) = 34.392 \text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation

$\Delta H_f^\circ(\text{K}_2\text{SO}_4, \text{l}, 298.15 \text{ K})$ is calculated from $\Delta H_f^\circ(\text{K}_2\text{SO}_4, \beta, 298.15 \text{ K})$ by adding the enthalpy of fusion, $\Delta_{\text{fus}}H^\circ$, and the difference in enthalpy, $H^\circ(1342 \text{ K}) - H^\circ(298.15 \text{ K})$, between the β-crystal and liquid.¹

Heat Capacity and Entropy

Enthalpies for K₂SO₄(l) have been measured by drop calorimetry by Shomate and Naylor (1358–1698 K),² Denielou *et al.* (1350–1550 K),³ and Rubinchik *et al.* (single point at 1344.84 K).⁴ A constant heat capacity of 46.15 cal·K⁻¹·mol⁻¹ is selected above a hypothetical glass transition at 800 K. Below the glass transition, the heat capacity is taken as that of the orthorhombic crystal.
 S°(K₂SO₄, l, 298.15 K) is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the K₂SO₄(cr, β) table for details.

Vaporization and Decomposition Data

K₂SO₄(l) can vaporize to the gaseous monomer K₂SO₄(g) or decompose according to K₂SO₄(l) = 2 K(g) + SO₂(g) + O₂(g). Vaporization pressures from the two processes are of comparable magnitude in the vicinity of the melting point.⁶ Recent experimental data for vaporization of K₂SO₄(cr)⁵ are in good agreement with dissociation pressures and the heat of reaction calculated from the JANAF Thermochemical Tables.¹ Molecular vaporization data are discussed on the K₂SO₄(g) table. T_{deg} = 2975 K is the calculated temperature at which the Gibbs energy difference is zero for the reaction K₂SO₄(l) = 2 K(g) + SO₂(g) + O₂(g). Decomposition to the oxides of potassium produces significantly lower decomposition pressures than decomposition to the metal. Significant decomposition can occur in the presence of water vapor according to K₂SO₄(l) + H₂O(g) = 2 KOH(g) + SO₂(g) + 1/2 O₂(g).

References

- ¹JANAF Thermochemical Tables: K₂SO₄(cr, α), K₂SO₄(cr, β), K₂SO₄(g), 6–30–78.
- ²C. H. Shomate and B. F. Naylor, *J. Amer. Chem. Soc.* **67**, 72 (1945).
- ³L. Denielou, Y. Fournier, J. P. Petitot, and C. Tequi, *C. R. Acad. Sci., Paris* **270**, 1854 (1975).
- ⁴S. M. Rubinchik, E. I. Banashek, V. A. Sokolov, and A. I. Fomin, *Russ. J. Phys. Chem.* **45**, 599 (1971).
- ⁵P. J. Ficalora, D. M. Uy, D. W. Muenow, and J. L. Margrave, *J. Amer. Ceram. Soc.* **51**, 574 (1968).
- ⁶K. H. Lau, D. Cubicciotti, and D. L. Hildenbrand, *J. Electrochem. Soc.* **126**, 490 (1979).

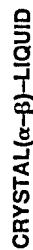
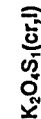
T/K	C _p ^o	S ^o	-(G ^o -H ^o (T))/T	H ^o -H ^o (T)	Δ _f H ^o	Δ _f G ^o	log K _r
0				0.			
100	131.319	211.505	211.505		-1393.668	-1286.278	223.351
200	131.666	212.319	211.508	0.243	-1393.685	-1285.612	223.845
298.15	147.649	252.455	216.872	14.213	-1401.191	-1248.498	163.037
300	160.733	286.831	227.505	29.663	-1402.022	-1210.215	126.430
400	172.577	317.148	239.966	46.309	-1401.359	-1171.892	102.022
500	186.368	344.790	252.992	64.259	-1399.257	-1133.794	84.605
600	199.619	370.547	266.094	83.563	-1395.792	-1096.092	71.567
800.000	199.619	370.547	266.094	83.563	GLASS <- -> LIQUID	TRANSITION	
800.000	201.460	370.547	266.094	83.563	GLASS <- -> LIQUID	TRANSITION	
900	201.460	394.276	279.044	103.709	-1444.670	-1057.804	61.393
1000	201.460	415.502	291.647	123.853	-1439.338	-1015.106	53.024
1100	201.460	434.703	303.793	144.001	-1592.120	-963.712	45.763
1200	201.460	452.232	315.443	164.147	-1585.116	-906.894	39.476
1300	201.460	468.338	326.594	184.293	-1578.196	-850.657	34.180
1342.000	201.460	474.763	331.132	192.754	- - - - -	BETA <- -> LIQUID	- - - - -
1400	201.460	483.287	337.260	204.439	-1571.353	-794.950	29.660
1500	201.460	497.187	347.464	224.585	-1564.582	-739.750	23.760
1600	201.460	510.189	357.232	244.731	-1557.880	-684.958	22.362
1700	201.460	522.402	366.592	264.877	-1551.245	-630.604	19.376
1800	201.460	533.917	375.571	285.022	-1544.678	-576.639	16.734
1900	201.460	544.809	384.195	305.168	-1538.178	-523.036	14.379
2000	201.460	555.143	392.486	325.314	-1531.747	-469.774	12.269
2100	201.460	564.972	400.467	345.460	-1525.387	-416.833	10.368
2200	201.460	574.344	408.159	365.606	-1519.101	-364.191	8.647
2300	201.460	583.299	415.581	385.752	-1512.892	-311.835	7.082
2400	201.460	591.873	422.749	405.898	-1506.763	-259.747	5.653
2500	201.460	600.097	429.680	426.044	-1500.719	-207.913	4.344
2600	201.460	607.999	436.387	446.190	-1494.762	-156.318	3.140
2700	201.460	615.602	442.883	466.336	-1488.898	-104.951	2.030
2800	201.460	622.929	449.185	486.482	-1483.129	-53.759	1.004
2900	201.460	629.978	455.239	506.628	-1477.463	-2.855	0.031
3000	201.460	636.828	461.237	526.774	-1471.903	47.901	-0.854

PREVIOUS: December 1971

CURRENT: June 1978

Potassium Sulfate (K₂SO₄)

K₂O₃S₁(l)



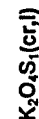
0 to 857 K crystal, alpha
857 to 1342 K crystal, beta
above 1342 to T_{em} K liquid

Refer to the single phase tables for the alpha, beta, liquid phases for details.

T/K	C_p^*	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa		$\log K_f$
		$S^\circ - (G^\circ - H^\circ(T_r))/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0	INFINITE	-25.436	-1427.199	-1427.199	INFINITE
100	79.195	61.609	-21.578	-1433.305	-1396.431	729.421
200	110.667	127.344	-11.915	-1436.295	-1358.245	354.737
298.15	131.319	175.544	0	-1437.706	-1319.595	231.188
300	131.666	176.357	0.243	-1437.723	-1318.862	229.634
400	147.649	216.494	14.233	-1445.229	-1278.152	166.909
500	160.733	250.870	29.663	-1446.060	-1236.272	129.153
600	172.527	281.186	46.309	-1445.397	-1194.353	103.978
700	186.368	308.829	64.259	-1443.295	-1152.659	86.012
800	199.619	334.580	83.558	-1439.835	-1111.361	72.564
857.000	207.169	348.575	95.151	—	—	—
857.000	184.000	358.437	103.603	—	—	—
900	187.485	367.530	111.590	-1480.836	-1069.890	62.095
1000	195.602	387.703	130.744	-1476.487	-1024.456	53.512
1100	203.761	406.729	150.713	-1629.446	-970.268	46.074
1200	211.878	424.807	171.494	-1621.806	-910.674	39.641
1300	219.995	442.087	193.089	-1613.438	-851.747	34.224
1342.000	223.384	449.136	202.400	—	—	—
1342.000	201.460	474.763	236.792	—	—	—
1400	201.460	483.287	248.477	-1571.353	-794.950	29.660
1500	201.460	497.187	318.105	-1564.582	-739.730	23.760
1600	201.460	510.189	328.769	-1557.880	-684.958	22.362
1700	201.460	522.402	340.688	-1551.245	-630.604	19.376
1800	201.460	533.917	351.106	-1544.678	-576.639	16.734
1900	201.460	544.809	361.017	-1538.178	-523.037	14.379
2000	201.460	555.143	370.467	-1531.747	-469.774	12.269
2100	201.460	564.972	379.497	-1525.387	-416.833	10.368
2200	201.460	574.344	388.142	-1519.101	-364.191	8.647
2300	201.460	583.299	396.434	-1512.892	-311.833	7.082
2400	201.460	591.873	404.400	-1506.763	-259.747	5.683
2500	201.460	600.097	412.064	-1500.719	-207.915	4.344
2600	201.460	607.999	419.449	-1494.762	-156.318	3.140
2700	201.460	615.602	426.574	-1488.898	-104.951	2.030
2800	201.460	622.929	433.457	-1483.179	-53.799	1.004
2900	201.460	629.998	440.113	-1477.663	-2.853	0.051
3000	201.460	636.828	446.557	-1471.903	47.901	-0.834

PREVIOUS:

CURRENT: June 1978



Potassium Sulfate (K₂O,S₁(g))

Potassium Sulfate (K₂SO₄)

IDEAL GAS

Potassium Sulfate (K₂SO₄)

$S^{\circ}(298.15\text{ K}) = 366.152 \pm 16.7\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ $\Delta H_f^{\circ}(0\text{ K}) = -1080.64 \pm 16.7\text{ kJ}\cdot\text{mol}^{-1}$ $\Delta H_f^{\circ}(298.15\text{ K}) = -1094.12 \pm 16.7\text{ kJ}\cdot\text{mol}^{-1}$

Vibrational Frequencies, Symmetries, and Degeneracies
 ν, cm^{-1} ν, cm^{-1} ν, cm^{-1}

A ₁	962 (1)	B ₁ [450] (1)	E 1098 (2)
	[458] (1)	B ₂ 1124 (1)	613 (2)
	[190] (1)	639 (1)	[230] (2)
		[262] (1)	[62] (2)

$\sigma = 4$

Ground State Quantum Weight: [11]

Point Group: D_{2h}

Bond Distances: S-O = 1.47 Å K-O = 1.45 Å

Bond Angles: O-S-O = 109.47° O-K-O = 58.67°

Product of the Moments of Inertia: $I_A I_B I_C = 2.626307 \times 10^{-112}\text{ g}^3\cdot\text{cm}^6$

Enthalpy of Formation

The adopted value of the enthalpy of formation is based on JANAF analyses of the vaporization data given below. Earlier data on the vaporization of K₂SO₄ is extremely discordant (for a review, refer to reference ¹⁰). Dissociation and other reactions play an important role in K₂SO₄ vaporization (refer to the K₂SO₄(l) table).

Torsion-effusion studies on the vaporization of K₂SO₄(g) by Lau *et al.*³ showed an orifice dependence which was reproduced in four separate runs. Plante *et al.*² did not observe this orifice size dependence in their effusion study, obtaining similar total pressures in two separate experiments. Calculated dissociation pressures were subtracted in both studies to obtain K₂SO₄(g) pressures. Similar results were obtained by Efimova and Gorokhov.¹ We have corrected the effusion data of Kosugi¹¹ for dissociation. The 3rd law enthalpy of sublimation from the three studies¹⁻³ are in very good agreement indicating similar K₂SO₄(g) pressures. The studies of Lau *et al.*³ and Efimova and Gorokhov¹ yield 2nd law enthalpy of sublimation (from K₂SO₄(cr, β)) some 6 kcal·mol⁻¹ greater than our calculated 3rd law enthalpy.

Lau *et al.*³ and Efimova and Gorokhov¹ also carried out mass spectrometric measurements of the K₂SO₄ ion intensity as a function of temperature. The 2nd law enthalpy of sublimation of Lau *et al.*³ obtained in two separate mass spectrometric experiments tend to corroborate their 2nd law enthalpy from the torsion-effusion measurements. The 2nd law enthalpy of Efimova and Gorokhov¹ as well as that of Ficalora *et al.*¹² are more in line with our 3rd law effusion values. Kosugi¹¹ did not observe the K₂SO₄ ion in his mass spectrometric experiments. The appearance potential of K₂SO₄ has been measured as 7.40 ± 0.5 eV,¹² 8.40 ± 0.3 eV³ and 8.0 eV.¹

We have discounted the transpiration experiments of Halstead¹³ and Dubois and Millet.¹⁴ The calculated 3rd law $\Delta H_f^{\circ}(298.15\text{ K})$ may have an uncertainty of 3 kcal·mol⁻¹ since the JANAF Gibbs energy functions are partially based on the estimated molecular constants of K₂SO₄(g). Our adopted ΔH_f° is based on a weighted average of the 3rd law results from.¹⁻³

Source	Method	Reaction*	T/K	Data Points	δS cal·K ⁻¹ ·mol ⁻¹	$\Delta H_f^{\circ}(298.15\text{ K})$, kcal·mol ⁻¹	$\Delta H_f^{\circ}(K_2SO_4, g, 298.15\text{ K})$, kcal·mol ⁻¹
Efimova ¹	effusion	A	1171-1331	equation	4.38	84.77	79.02 ± 0.11
			1180-1274	37	5.18	85.36	78.93 ± 0.45
Lau <i>et al.</i> ³	torsion-effusion	A	1166-1322	26	-1.42 ± 0.8	77.03 ± 0.9	78.78 ± 0.42
			1196-1321	15	-0.76 ± 2.0	77.87 ± 2.0	78.83 ± 0.51
Halstead	effusion	A	1180-1340	equation	1.07	75.75	74.39 ± 0.15
			1409-1530	12	2.70 ± 2.8	73.67 ± 4.2	69.66 ± 0.76
Kosugi ¹¹	effusion	B	1171-1331	?	—	78.0 ± 1.0	-262.4 ± 2
			1183-1248	9	—	84.12 ± 2.02	-256.28 ± 2.0
Lau <i>et al.</i> ³	mass spec	A	1180-1314	10	—	81.96 ± 0.40	-258.44 ± 1.5
			1080-1230	?	—	79.8 ± 2.0	-260.6 ± 4
Ficalora ¹²	mass spec	A)					
		B)					

*Reactions: A) K₂SO₄(cr, β) = K₂SO₄(g)

Heat Capacity and Entropy

The adopted structure (D_{2h} symmetry) is based on the high temperature electron diffraction study of Spiridonov and Lutoshkin.⁵ This symmetry is supported by the similar work of Ugarov *et al.*⁴ on Cs₂SO₄ and the IR and Raman study of Atkins and Gingerich⁶ on K₂SO₄ and Na₂SO₄. The molecule can be pictured as having a central sulfur atom surrounded at the corners of a tetrahedron by four oxygen atoms with bridging potassium atoms between two pairs of oxygens forming two planar mutually perpendicular KO₂S rings. The sulfate core is fairly

T/K	C _p ^o	S ^o - (G ^o - H ^o (T))/T	H ^o - H ^o (T)	ΔH ^o	log K _r
0	0	INFINITE	INFINITE	0	INFINITE
100	64.770	273.209	-22.463	-1080.636	-1080.636
200	90.384	326.456	-17.647	-1085.784	-1070.071
250	100.439	347.734	-9.818	-1090.608	-1052.380
298.15	108.730	366.152	-5.041	-1094.116	-1042.597
300	109.023	366.154	0.201	-1094.116	-1032.835
350	116.277	367.509	5.839	-1100.439	-1021.853
400	122.342	370.604	11.869	-1104.063	-1010.439
450	127.380	374.713	18.056	-1105.903	-998.632
500	131.555	379.416	24.533	-1107.600	-986.618
600	137.903	389.688	38.025	-1110.091	-962.173
700	142.345	400.317	52.050	-1111.914	-937.369
800	145.525	410.835	66.452	-1113.351	-912.333
900	147.859	421.041	81.227	-1117.008	-886.050
1000	149.612	430.851	96.005	-1167.636	-854.758
1100	150.956	440.239	111.036	-1325.533	-814.251
1200	152.006	449.208	126.186	-1321.524	-767.860
1300	152.842	456.564	141.430	-1321.507	-721.636
1400	153.515	463.017	156.749	-1319.491	-675.568
1500	154.007	468.527	172.129	-1317.486	-629.644
1600	154.523	473.775	187.559	-1315.500	-583.853
1700	154.904	478.665	203.031	-1313.539	-538.185
1800	155.226	483.319	218.538	-1311.610	-492.632
1900	155.500	487.729	234.075	-1309.720	-447.185
2000	155.736	491.933	249.637	-1307.873	-401.836
2100	155.940	495.945	265.221	-1306.075	-356.579
2200	156.117	499.773	280.824	-1304.332	-311.405
2300	156.272	503.428	296.444	-1302.649	-266.310
2400	156.409	506.910	312.078	-1301.032	-221.288
2500	156.529	509.257	327.725	-1299.487	-176.330
2600	156.637	511.471	343.383	-1298.017	-131.433
2700	156.731	513.558	359.042	-1296.610	-86.591
2800	156.810	515.519	374.729	-1295.263	-41.798
2900	156.886	517.362	390.415	-1293.974	3.043
3000	156.966	519.099	406.108	-1292.742	47.656
3100	157.029	520.736	421.808	-1291.566	92.329
3200	157.078	522.277	437.514	-1290.444	137.067
3300	157.119	523.725	453.225	-1289.366	181.863
3400	157.157	525.082	468.942	-1288.332	226.718
3500	157.231	526.351	484.663	-1287.345	271.633
3600	157.272	527.536	500.388	-1286.400	316.616
3700	157.299	528.636	516.117	-1285.500	361.665
3800	157.343	529.649	531.850	-1284.645	406.777
3900	157.375	530.579	547.586	-1283.823	451.950
4000	157.404	531.426	563.325	-1283.035	497.183
4100	157.421	532.191	579.066	-1282.281	542.474
4200	157.427	532.874	594.811	-1281.561	587.820
4300	157.421	533.475	610.558	-1280.874	633.222
4400	157.403	534.000	626.307	-1280.220	678.679
4500	157.373	534.457	642.058	-1279.592	724.192
4600	157.332	534.846	657.812	-1279.000	769.761
4700	157.281	535.167	673.567	-1278.444	815.284
4800	157.221	535.421	689.324	-1277.923	860.758
4900	157.157	535.608	705.082	-1277.436	906.181
5000	157.099	535.734	720.842	-1276.982	951.554
5100	157.033	535.801	736.604	-1276.564	996.877
5200	156.956	535.808	752.367	-1276.181	1042.150
5300	156.869	535.754	768.131	-1275.833	1087.373
5400	156.772	535.639	783.897	-1275.520	1132.546
5500	156.666	535.464	799.663	-1275.242	1177.669
5600	156.552	535.229	815.431	-1275.000	1222.742
5700	156.431	534.934	831.200	-1274.792	1267.765
5800	156.302	534.579	846.969	-1274.618	1312.738
5900	156.167	534.164	862.740	-1274.478	1357.661
6000	156.026	533.690	878.512	-1274.362	1402.534

PREVIOUS: June 1978 (1 atm)

CURRENT: June 1978 (1 bar)

K₂S₁(cr)Potassium Sulfide (K₂S)M_r = 110.2566

CRYSTAL

Potassium Sulfide (K₂S)

S⁰(298.15 K) = 115.06 ± 16.7 J·K⁻¹·mol⁻¹
 T_m = 1050 ± 10 K (diffuse lambda transition)
 T₀₂ = 1221 ± 10 K

Δ_fH⁰(298.15 K) = -376.56 ± 12.6 kJ·mol⁻¹
 Δ_{sub}H⁰ = 0 kJ·mol⁻¹
 Δ_{sub}H⁰ = 16.150 ± 0.17 kJ·mol⁻¹

Enthalpy of Formation

Experimental measurements leading to the enthalpy of formation of K₂S(cr) are summarized below.

Source	Reaction	Δ _f H ⁰ (298.15 K), kcal·mol ⁻¹
Sabatier ¹	Δ _{sub} H ⁰ K ₂ S(cr) and K(cr); Δ _{sub} H ⁰ KOH(aq) + H ₂ S(aq)	-103.4
Rengade and Costeau ²		-87.3
Letoffe <i>et al.</i> ³	H ₂ SO ₄ (aq, 1100 H ₂ O) + K ₂ S(cr) = K ₂ SO ₄ (aq, 1100 H ₂ O) + H ₂ (g)	-92.1 ^a
a. The authors' value of -91.1 ± 0.9 kcal·mol ⁻¹ is changed by new Δ _f H ⁰ (298.15 K) values for H ₂ SO ₄ (aq, 1100 H ₂ O), K ₂ SO ₄ (cr) and H ₂ (g). ^{4,5}		

Since Sabatier himself has expressed reservations because of impure material, we eliminate his value and adopt the average of the other two values, Δ_fH⁰(K₂S, cr, 298.15 K) = -90 ± 3 kcal·mol⁻¹.

Heat Capacity and Entropy

The heat capacity is taken from the drop calorimetry of Dworkin and Bredig (384 to 1260 K).⁶ Between 298 and 820 K, the observed enthalpy differences and the constraint of passing through zero at 298.15 K are fit by a linear least squares technique; C_p⁰ = 15.99 + 6.22 × 10⁻³ T cal·K⁻¹·mol⁻¹ (298-820 K). The heat capacity in the observed diffuse lambda transition region, 820-1100 K, was adjusted to properly reproduce the observed enthalpies. The sharp heat capacity maximum occurs at 1050 K⁶ and 46.60 cal·K⁻¹·mol⁻¹. From 1100 K to the melting point, 1221 K,⁷ the heat capacity was found to be constant at 46.60 cal·K⁻¹·mol⁻¹.

Freeman⁸ has estimated S⁰(K₂S, cr, 298.15 K) = 27 cal·K⁻¹·mol⁻¹; Voronin⁹ also has estimated 27 cal·K⁻¹·mol⁻¹. Kelley's additive entropy constants give 28.0 We adopt S⁰(K₂S, cr, 298.15 K) = 27.5 ± 4 cal·K⁻¹·mol⁻¹.

Transition and Fusion Data

A crystal II to crystal I transition at 419.6 K with an enthalpy change of 0.085 kcal·mol⁻¹ has been listed¹⁰ from Bridgman. However, West¹² found no change in the x-ray powder diffraction pattern over the 298-473 K range. Although not definitive because of the small heat change listed, the drop calorimetric enthalpy measurements of Dworkin and Bredig⁶ do not show this transition. Therefore, we do not indicate any solid state transition at 419.6 K.

The diffuse lambda transition has been discussed above.

A melting point of 1221 K was determined by thermal analysis (cooling curves) of the K-K₂S system by Dworkin and Bredig.⁷ This is considerably higher than earlier values of 1108 K¹¹ and 1185 K,¹⁴ but it is confirmed by their drop calorimetric measurements.⁶ A melting point of 1221 ± 10 K is adopted with Δ_{sub}H⁰ = 3.86 ± 0.04 kcal·mol⁻¹.

References

- ¹P. Sabatier, *Annls. Chim. Phys. Ser. 5*, **22**, 5 (1881).
- ²E. Rengade and N. Costeau, *Compt. rend.* **158**, 946 (1914), and *Bull. Soc. Chim. Fr.* **15**, 717 (1914).
- ³J. M. Letoffe, R. D. Joly, J. Thoury, G. Perathon, and J. Bousquet, *J. Chem. Phys. Physicochim. Biol.* **71**, 427 (1974), and J. M. Letoffe, Doctorate Thesis, Université Claude Bernard Lyon I, (1975).
- ⁴U. S. Nat. Bur. Stand. Tech. Note 270-3, 264 pp. (1968).
- ⁵JANAF Thermochemical Tables: K₂SO₄(cr), 12-31-71, H₂S(g), 6-30-77.
- ⁶A. S. Dworkin and M. A. Bredig, *J. Phys. Chem.* **72**, 1277 (1968).
- ⁷A. S. Dworkin and M. A. Bredig, *J. Phys. Chem.* **71**, 764 (1967).
- ⁸R. D. Freeman, Oklahoma State University, Department of Chemistry, Research Foundation Report No. 60, (1962).
- ⁹G. F. Voronin, *Russ J. Phys. Chem.* **44**, 1717 (1970).
- ¹⁰P. W. Bridgman, *Proc. Am. Acad. Arts Sci.* **51**, 53 (1915).
- ¹¹C. D. West, *Z. Krist.* **88**, 97 (1934).
- ¹²O. Kubaschewski, E. L. Evans and C. B. Alcock, "Metallurgical Thermochemistry," 4th ed., Pergamon Press, Oxford, (1967).
- ¹³J. Goubeau, H. Kolb, and H. G. Krall, *Z. anorg. allg. Chem.* **246**, 45 (1938).

PREVIOUS.

CURRENT: March 1978

Potassium Sulfide (K₂S)K₂S₁(cr)

Potassium Sulfide (K₂S)

M_r = 110.2566 Potassium Sulfide (K₂S)

K₂S_l(cr,l)

CRYSTAL-LIQUID

0 to 1050 K*crystal
1050 to 1221 K crystal
above 1221 K liquid

Refer to the individual tables for details.

*There is a diffuse transition at 1030 K.

T/K	C _p ^a	Enthalpy Reference Temperature = T _r = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K _r
		J·K ⁻¹ ·mol ⁻¹	S° - [G° - H°(T _r)]/T	H° - H°(T _r)	Δ _r H°	
0						
100						
200						
250						
298.15	74.684	115.060	115.060	0.	-376.560	-362.745
300	74.726	115.522	115.061	0.138	-376.573	-362.659
400	77.320	118.023	118.023	7.741	-384.524	-356.897
500	79.914	123.702	123.702	15.602	-386.806	-349.730
600	82.508	169.706	130.167	23.723	-388.349	-342.158
700	85.144	182.621	136.757	32.105	-389.306	-334.377
800	87.738	194.161	143.224	40.749	-389.826	-326.490
900	103.554	205.100	149.486	50.053	-442.745	-317.488
1000	156.063	218.274	155.672	62.602	-438.078	-303.773
1050.000	194.982	226.816	158.850	71.364		
1050.000	194.985	226.816	158.850	71.364		
1100	142.340	234.558	162.127	79.675	-586.914	-281.577
1200	142.340	246.943	168.686	93.908	-578.724	-254.180
1221.000	142.340	249.413	170.053	96.898		
1221.000	100.960	262.640	170.053	113.048		
1300	100.960	268.969	175.874	121.024	-557.669	-278.408
1400	100.960	276.451	182.794	131.120	-553.649	-263.231
1500	100.960	283.417	189.273	141.216	-549.646	-178.341
1600	100.960	289.932	195.363	151.312	-545.660	-153.717
1700	100.960	296.053	201.107	161.408	-541.691	-129.343
1800	100.960	301.824	206.544	171.504	-537.742	-105.201
1900	100.960	307.282	211.704	181.600	-533.813	-81.278
2000	100.960	312.461	216.613	191.696	-529.907	-57.562
2100	100.960	317.387	221.296	201.792	-526.026	-34.040
2200	100.960	322.084	225.771	211.888	-522.174	-10.702
2300	100.960	326.571	230.057	221.984	-518.353	12.461
2400	100.960	330.868	234.168	232.080	-514.569	35.458
2500	100.960	334.990	238.119	242.176	-510.825	58.299
2600	100.960	338.949	241.972	252.272	-507.125	80.991
2700	100.960	342.760	245.586	262.368	-503.470	103.541
2800	100.960	346.431	249.123	272.464	-499.862	125.957
2900	100.960	349.974	252.540	282.560	-496.350	148.246
3000	100.960	353.397	255.845	292.656	-492.887	170.414

PREVIOUS.

CURRENT- March 1978

Potassium Sulfide (K₂S)

K₂S_l(cr,l)

Potassium

Continued from page 1469

- ¹⁴W. Edmondson and C. A. Egerton, Proc. Roy. Soc. (London) **A113**, 520 (1927).
¹⁵J. Weiler, Ann. Physik [5] **1**, 361, 33 (1932).
¹⁶H. Mayer, Z. Physik **69**, 786 (1931).
¹⁷K. Neumann and E. Volker, Z. Physik. Chem. **161**, 33 (1932).
¹⁸J. F. Walling, J. Phys. Chem. **67**, 1380 (1963).
¹⁹M. M. Makansi, M. Maasem, *et al.*, J. Phys. Chem. **60**, 128 (1956).
²⁰U. Buck and H. Pauly, Z. Physik. Chem. (Frankfurt) **44**, 345 (1965).
²¹D. P. Stone, C. P. Ewing, *et al.*, J. Chem. Eng. Data **11**, 315 (1966).
²²D. V. Rigney, S. M. Kapelner, and R. E. Cleary, U. S. AEC Rept. TTM-810 (1965).
²³Yu. K. Vinogradov and L. D. volyak, Teplofiz. vys. Temp. **4**, 50 (1966).
²⁴P. Y. Achmeier, U. S. AEC Rept. AGN-8141, (1965).
²⁵E. Shipil'rain, E. E. Tozku, and V. A. Sherishevsku, Teplofiz. Vep. Temp. **6**, 924 (1968).
²⁶K. J. Bowles, NASA Tech. Note D-4535, (1968).
²⁷Ya. I. Gerasimov, G. F. Vorontin and N. T. Shiu, J. Chem. Thermodynamics **1**, 425 (1969); Zhur. Fiz. Khim. **41**, 1468 (1968).
²⁸E. E. Shipil'rain and E. V. Nikanorov, Teplofiz. Svoistva Gasov Mater. Vsih Teplofiz. Konf. Svoistvam. Vshchister Vyz. Temp. (1968), Mosk. "Nauka," 141 (1970).
²⁹H. E. J. Schins, R. W. M. van Wijk and b. Dorpema, Z. Metallkunde **62**, 330 (1971).
³⁰C. F. Bonilla, U. S. AEC Rept. ORNL-3605, **1**, 286 (1964).
³¹A. Roeder and W. Morawitz, Z. Elektrochem. **60**, 431 (1956).
³²N. S. Kondrat'ev and I. F. Parfent'eva, Teplo-massopretnos v odno-z-dvukhriznykh sudakh, Moskov, "Nauka," 19 (1971).
³³C. Corliss and J. Sugar, J. Phys. Chem. Ref. Data **8**, 1109 (1979).
³⁴J. R. Downey, Jr., The Dow Chemical Company, Rept. AFOSR-TR-78-0960, Contract No. F44620-75-0048, (1978).
³⁵C. H. Shonate and B. F. Naylor, J. Amer. Chem. Soc. **67**, 72 (1945).
³⁶A. S. Dworkin and M. A. Bredig, J. Phys. Chem. **74**, 3403 (1970).
³⁷L. Denielou, Y. Fournier, J. P. Pettiet, and C. Tequi, C. R. Acad. Sci., Paris **270**, 1854 (1970).
³⁸S. M. Rubinchik, E. I. Banashek, V. A. Sokolov, and A. I. Fomin, Russ. J. Phys. Chem. **45**, 599 (1971).

Continued from page 1481

- Continuation of discussions of selected K species
- ²⁴M. T. Robinson, J. Phys. Chem. **62**, 925 (1958).
²⁵C. W. F. T. Pistorius and E. Rapoport, J. Phys. Chem. Solids **30**, 195.
- Continued from page 1485
- rigid while the metal atoms undergo large amplitude motions. The internuclear distances of 1.47 Å for S-O and 2.45 Å for K-O are from²⁴ as are the O-S-O and O-K-O angles. The principal moments of inertia are $I_A = 15.3096 \times 10^{-39}$ and $I_B = I_C = 130.9758 \times 10^{-39}$ g-cm².
 Atkins and Gincerich²⁵ have observed the infrared and Raman spectra of K₂SO₄ and Na₂SO₄ isolated in oxygen and nitrogen matrices at 12 K. Five of the eleven fundamental frequencies were observed in this work. Good agreement exists between these observations and the frequencies adopted by Gurvich *et al.*⁶ The two other sulfate-ion group fundamentals are taken from the Raman study of Davies and Sandford.⁹ The low-frequency fundamentals involving the metal atoms are taken from the infrared study of Belyaeva *et al.*⁸ These authors observed the spectra of K₂SO₄, Rb₂SO₄, and Cs₂SO₄ isolated in Ar, Kr, and Xe matrices at 4.2 K. Uncertainties in the location of the gas phase frequencies may contribute 4 cal-K⁻¹ mol⁻¹ to S⁰(298.15 K).
- References
¹A. G. Effimova and L. N. Gorokhov, Teplofiz. Vys. Temp. **16**, 1195 (1978); L. N. Gorokhov, High Temperature Technology, Proc. Third International Symposium on High Temperature Technology (1967) Butterworths, London; L. N. Gorokhov and A. G. Effimova Annual Report, Institute for High Temperatures, Academy of Sciences, USSR, 1975, "Nauka," (1976).
²E. R. Plante, C. D. Olson, and T. Negas, U. S. Nat. Bur. Stand., personal communication, (1978).
³K. H. Lau, D. Cubicciotti, and D. L. Hildenbrand, J. Electrochem. Soc. **126**, 490 (1979).
⁴V. V. Ugarov, Yu. S. Ezhov, and N. G. Rambidi, J. Mol. Struct. **25**, 357 (1975).
⁵V. P. Spindonov and B. I. Lutoshkin, Vestn. Mosk. Univ. **11**, 509 (1970) (English trans. NASA TT F 16199).
⁶L. V. Gurvich, O. V. Dorofeeva, and V. S. Yungman, Proceedings of the Conference on High Temperature Science related to Open Cycle Coal-Fuel MHD Systems, Argonne National Lab. Report ANL-77-21 (1977).
⁷R. M. Atkins and K. A. Gimerich, Chem. Phys. Lett. **53**, 347 (1978).
⁸A. A. Belyaeva, M. I. Dworkin, and L. D. Shcherba, Opt. Spectroscopy **38**, 170 (1975), **38**, 291 (1975); **43**, 114 (1977).
⁹J. E. D. Davies and W. F. Sandford, J. Chem. Soc. **1912** (1975).
¹⁰I. Eliezer and R. A. Howald, J. Chem. Phys. **65**, 3053 (1976).
¹¹T. Kosugi, Bull. Chem. Soc. Japan **45**, 15 (1972), Kogyo Kagaku Zasshi **70**, 2089 (1967).
¹²P. J. Ficalora, D. M. Uy, D. W. Muenow, and J. L. Margrave, J. Amer. Ceram. Soc. **51**, 574 (1968).
¹³W. D. Halstead, Trans. Faraday Soc. **66**, 1966 (1970).
¹⁴J. Dubois and J. Millet, C. R. Acad. Sci. **266**, 852 (1968).