REFERENCE STATE

0	to 2130		K	crystal
2130	to 2952.078		K	liquid
above		2952.078	K	ideal monatomic gas

Refer to the individual tables for details.

A_r = 51.996 Chromium (Cr) Cr_1(ref)

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

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−4.057	0.	0.	0.
100	9.963	4.286	41.746	−3.746	0.	0.	0.
200	19.860	14.869	25.680	−2.162	0.	0.	0.
298.15	23.434	23.618	23.618	0.	0.	0.	0.
300	23.472	23.764	23.619	0.043	0.	0.	0.
311.500	23.681	24.651	23.641	0.315	C_p LAMBDA MAXIMUM TRANSITION		
311.500	23.681	24.654	23.641	0.316			
400	25.230	30.765	24.562	2.481	0	0.	0.
500	26.631	36.553	26.398	5.078	0	0.	0.
600	27.719	41.508	28.513	7.797	0	0.	0.
700	28.577	45.846	30.686	10.612	0	0.	0.
800	29.434	49.715	32.827	13.511	0.	0.	0.
900	30.501	53.241	34.902	16.505	0.	0.	0.
1000	31.861	56.523	36.901	19.621	0	0.	0.
1100	33.472	59.634	38.828	22.887	0.	0.	0.
1200	35.187	62.618	40.687	26.318	0.	0.	0.
1300	37.116	65.511	42.485	29.933	0	0.	0
1400	39.125	68.334	44.231	33.744	0	0.	0.
1500	41.200	71.104	45.931	37.760	0.	0.	0.
1600	43.329	73.831	47.589	41.986	0.	0.	0
1700	45.501	76.523	49.212	46.427	0	0.	0
1800	47 706	79.186	50.804	51.087	0.	0.	0.
1900	49.944	81.825	52.367	55.970	0.	0.	0.
2000	52.204	84.444	53.905	61.077	0.	0.	0.
2100	54 488	87.046	55.422	66.411	0	0.	0
2130.000	55.174	87.824	55.873	68.056	CRYSTAL <- -> LIQUID TRANSITION		
2130.000	39.330	97.449	55.873	88.558			
2200	39.330	98.721	57.216	91.311	0.	0	0
2300	39.330	100.469	59.059	95.244	0.	0.	0.
2400	39.330	102.143	60.819	99.177	0.	0.	0.
2500	39.330	103.749	62.505	103.110	0.	0.	0.
2600	39.330	105.291	64.121	107.043	0.	0.	0.
2700	39.330	106.775	65.673	110.976	0.	0.	0.
2800	39.330	108.206	67.167	114.909	0.	0.	0.
2900	39.330	109.586	68.606	118.842	0.	0.	0.
2952.078	39.330	110.286	69.335	120.890	LIQUID <- -> IDEAL GAS FUGACITY = 1 bar		
2952.078	30.533	225.302	69.335	460.427			
3000	30.788	225.796	71.830	461.897	0.	0.	0
3100	31.302	226.814	76.813	465.001	0.	0.	0.
3200	31.796	227.815	81.517	468.156	0.	0.	0.
3300	32.275	228.801	85.965	471.360	0.	0.	0.
3400	32.745	229.772	90.180	474.611	0.	0.	0.
3500	33.212	230.728	94.182	477.909	0.	0.	0
3600	33.680	231.670	97.988	481.253	0.	0.	0.
3700	34.156	232.599	101.614	484.645	0.	0.	0.
3800	34.646	233.516	105.073	488.085	0.	0.	0
3900	35.157	234.423	108.378	491.575	0.	0.	0.
4000	35.692	235.320	111.540	495.117	0.	0.	0.
4100	36.260	236.208	114.570	498.715	0.	0.	0.
4200	36.864	237.089	117.477	502.370	0.	0.	0.
4300	37.511	237.964	120.269	506 089	0.	0.	0.
4400	38.205	238.834	122.954	509.874	0.	0.	0.
4500	38.954	239.701	125.538	513.732	0.	0.	0.
4600	39.760	240.566	128.030	517.667	0.	0.	0.
4700	40.632	241.430	130.433	521.686	0.	0.	0.
4800	41.572	242.295	132.755	525.795	0.	0.	0.
4900	42.587	243.163	134.999	530.003	0.	0.	0.
5000	43.681	244.034	137.171	534.315	0.	0.	0.
5200	44.964	245.697	141.308	542.822	0.	0.	0.
5400	47.221	247.435	145.206	552.036	0.	0.	0.
5600	49.697	249.197	148.889	561.724	0.	0.	0.
5800	52.370	250.986	152.378	571.925	0.	0.	0.
6000	55.230	252.809	155.696	582.682	0.	0.	0.

PREVIOUS: June 1973 (1 atm) CURRENT June 1973 (1 bar)

Chromium (Cr) Cr_1(ref)

Chromium (Cr) CRYSTAL $A_r = 51.996$

$S°(298.15\ K) = 23.618 \pm 0.21\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{trs} = 311.5\ K$
$T_{fus} = 2130 \pm 20\ K$

$\Delta_f H°(0\ K) = 0\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ{\cdot}mol^{-1}$
$\Delta_{trs} H° = 0.0008\ kJ{\cdot}mol^{-1}$
$\Delta_{fus} H° = 20.5 \pm 4.2\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The heat capacity values for $T \leq 10$ K are chosen to be the same as those adopted by Hultgren *et al.*[1] A graphical integration of these $C_p°$ data yields $S°(10\ K) = 0.005\ kcal{\cdot}mol^{-1}$ and $H°(10\ K)-H°(0\ K) = 0.0252\ cal{\cdot}mol^{-1}$. These data also match well with the $C_p°$ studies of Clusius and Franzosini.[2] The adopted $C_p°$ values are based on the following studies.

Source	Points	Method	T/K
2	76	$C_p°$	14.10–274.43
3	23	$C_p°$	56.1 –291.1
4	Smooth	$C_p°$	60–300
5	Graph	$C_p°$	268–324
6	Smooth	$C_p°$	273–1073
7	Smooth	drop	400–1500
8	48	drop	1267.2108
9	17	drop	303–1884
10	Smooth	$C_p°$	320–1800
11	26	drop	673–1339

The adopted $C_p°$ values are obtained primarily by graphical techniques to ensure smoothness of the curve and a reasonable representation of the sometimes diverse results. A $\Delta C_p° = 0$ is also adopted across T_{trs}. Below 200 K, there is excellent agreement between three independent studies.[2-4] Above 200 K these three studies drift apart by at most 0.06 kcal·mol^{-1}. Above 298 K, there are considerable differences in the various sets of data, differences of the order of 0.2 kcal·mol^{-1} being typical. In terms of enthalpy, the data of Jaeger and Rosenbohm[11] deviates from the adopted values by +150 to +350 cal·mol^{-1}; the data of Lucks and Deem[9] by 0 to −450 cal·mol^{-1}; the data of Hultgren and Land[7] by −13 to +60 cal·mol^{-1}; and the data of Conway and Hein[8] by −190 to +250 cal·mol^{-1} Surprisingly the enthalpy study by Kirillin *et al.*[12] yields enthalpies which are crudely 2 kcal·mol^{-1} less than the adopted values at 2000 K.

Fusion Data

Refer to the liquid table for details.

Transition Data

Beaumont *et al.*[5] measured the heat capacity of 99.998% pure Cr in the region 268–324 K. The detailed $C_p°$ measurements gave evidence of a lambda–type anomaly, the maximum occurring at 311.5 K. Beaument *et al.*[5] estimated the heat associated with this transition to be 1.4 cal·mol^{-1}. Garnier and Salamon[13] used an extension of the ac calorimetric method to determine latent heat and heat capacity simultaneously. They concluded that annealing the Cr sample decreases the transition temperature and sharpens the peak. They also concluded that the transition was first order with a latent heat of 0.19 ± 0.04 cal·mol^{-1} at a transition temperature of 311.5 K. Garnier and Salamon[13] calculated a latent heat of 0.23 ± 0.05 cal·mol^{-1} and 0.25 ± 0.08 cal·mol^{-1} from expansivity data and neutron–diffraction data, respectively. Sze and Meaden[14] observed a large step in specific heat measurements (50%) and estimated a latent heat of 0.47 cal·mol^{-1}.

We adopt $T_{trs} = 311.5$ K and $\Delta_{fus}H° = 0.0002\ kcal{\cdot}mol^{-1}$ based on the work by Garnier and Salamon.[13] In addition we adopt $\Delta C_p° = 0$ across the transition. The nature of the transition is not understood at this time.

Sublimation Data

Refer to the ideal gas table for details.

References

[1] R. Hultgren, R. L. Orr, and K. K. Kelley, Supplement to Selected Values of Thermodynamic Properties of Metals and Alloys, Cr table, (October 1966).
[2] K. Clusius and P. Franzosini, Z. Naturforsch. 17a, 522 (1962).
[3] C. T. Anderson, J. Amer. Chem. Soc. 59, 488 (1937).
[4] G. I. Kalishevich, P. V. Gel'd, and R. P. Krentsis, Russ. J. Phys. Chem. 39, 1602 (1965).
[5] R. H. Beaumont, H. Chihara, and J. A. Morrison, Phil. Mag. 5, 188 (1960).
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Chromium (Cr) $Cr_1(cr)$

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

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−4.057	0.	0.	0.
100	9.963	4.286	41.746	−3.746	0.	0.	0.
200	19.860	14.869	25.680	−2.162	0.	0.	0.
250	22.298	19.590	23.998	−1.102	0.	0.	0.
298.15	23.434	23.618	23.618	0.	0.	0.	0.
300	23.472	23.764	23.619	0.043	0.	0.	0.
311.500	23.681	24.651	23.641	0.315	—— C_p LAMBDA MAXIMUM TRANSITION ——		
311.500	23.681	24.654	23.641	0.316			
350	24.393	27.453	23.908	1.240	0.	0.	0.
400	25.230	30.765	24.562	2.481	0.	0.	0.
450	25.983	33.781	25.421	3.762	0.	0.	0.
500	26.631	36.553	26.398	5.078	0.	0.	0.
600	27.719	41.508	28.513	7 797	0.	0.	0.
700	28.577	45.846	30.686	10.612	0.	0.	0.
800	29.434	49.715	32.827	13.511	0.	0.	0.
900	30.501	53.241	34.902	16.505	0.	0.	0.
1000	31.861	56.523	36.901	19.621	0.	0.	0.
1100	33.472	59.634	38.828	22.887	0.	0.	0.
1200	35.187	62.618	40.687	26.318	0.	0.	0.
1300	37.116	65.511	42.485	29.933	0.	0.	0.
1400	39.125	68.334	44.231	33.744	0.	0.	0.
1500	41.200	71.104	45.931	37.760	0.	0.	0.
1600	43.329	73.831	47.589	41.986	0.	0.	0.
1700	45.501	76.523	49.212	46.427	0.	0.	0.
1800	47.706	79.186	50.804	51.087	0.	0.	0.
1900	49.944	81.825	52.367	55.970	0.	0.	0.
2000	52.204	84.444	53.905	61.077	0.	0.	0.
2100	54.488	87.046	55.422	66.411	0.	0.	0.
2130.000	55.174	87.824	55.873	68.056	– – – CRYSTAL <– –> LIQUID – – –		
2200	56.785	89.634	56.918	71.975	−19.336	0.655	−0.016
2300	59.099	92.209	58.397	77.769	−17.475	1.523	−0.035
2400	61.425	94.774	59.859	83.795	−15.382	2.305	−0.050
2500	63.764	97.328	61.307	90.055	−13.055	2.995	−0.063
2600	66.111	99.875	62.741	96.548	−10 495	3.587	−0.072
2700	68.467	102.414	64.163	103.277	−7.699	4.076	−0.079
2800	70.831	104.947	65.575	110.242	−4.667	4.458	−0.083

PREVIOUS: CURRENT. June 1973

Chromium (Cr) $Cr_1(cr)$

Chromium (Cr) LIQUID $A_r = 51.996$ Chromium (Cr) $Cr_1(l)$

$S°(298.15\ K) = [36.205]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_f H°(298.15\ K) = [26.068]\ kJ{\cdot}mol^{-1}$

$T_{fus} = 2130 \pm 20\ K$ $\Delta_{fus}H° = 20.5 \pm 4.2\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

The enthalpy of formation of Cr(l) at 298.15 K is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(2130\ K)–H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The heat capacity for Cr(l) is estimated as $9.4\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ by analogy with other monatomic metals The same value was adopted by Hutgren *et al.*[1] A glass transition is assumed at 1350 K. Below 1350 K, the $C_p°$ values are those of the crystal. The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

The value for the enthalpy of melting is adopted as $\Delta_{fus}H° = 4.9 \pm 1.0\ kcal{\cdot}mol^{-1}$. This value is calculated from $\Delta_{fus}S° = 2.3\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. This estimated entropy of melting is consistent with the recently accepted $\Delta_{fus}S°$ values for V[2], 2.49 cal K – mol^{-1}), Nb[2], 2.33 cal·K^{-1}·mol^{-1}), and Ta[2], 2.68 cal·K^{-1}·mol^{-1}). This is in contrast to a value of $\Delta_{fus}S° = 1.9\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ used by Hultgren *et al.*[1]

The melting temperature is adopted as $T_{fus} = 2130$ K as was chosen by Hultgren *et al.*[1] Values reported in the literature are:

Source	Year	T, K
[3]	1949	2133
[4]	1951	2118 ± 10
[5]	1952	2176 ± 10
[6]	1959	2122

Vaporization Data

The value for T_{vap} calculated as the temperature for which the Gibbs energy for the reaction Cr(l) = Cr(g) is zero. The difference in the enthalpy of formation of Cr(l) and Cr(g) at T_{vap} is $\Delta_{vap}H°$.

References

[1] R. Hultgren, R. L. Orr, and K. K. Kelley, Supplement to Selected Values of Thermodynamic Properties of Metals and Alloys, Cr table, (October 1966).

[2] JANAF Thermochemical Tables: V(cr), 6–30–73; Nb(cr) and Ta(cr), 12–31–72.

[3] S. J. Carlile, J. W. Christian, and W. Hume-Rothery, J. Inst. Metals 76, 169 (1949).

[4] H. T. Greenaway, S. T. M. Johnstone, and M. K. McQuillan, J. Inst. Metals 80, 109 (1951).

[5] D. S. Bloom, J. W. Putman, and N. J. Grant, J. Metals 4, 626 (1952).

[6] C. W. Haworth and W. Hume-Rothery, J. Inst. Metals 87, 265 (1959).

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

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0							
100							
200							
250							
298.15	23.434	36.205	36.205	0.	26.068	22.316	−3.910
300	23.472	36.350	36.205	0.043	26.068	22.292	−3.881
350	24.393	40.036	36.495	1.240	26.067	21.663	−3.233
400	25.230	43.349	37.148	2.481	26.067	21 034	−2.747
450	25.983	46.365	38.007	3.761	26.067	20.405	−2.369
500	26.631	49.137	38.983	5.077	26.067	19.775	−2.066
600	27.722	54.092	41.098	7.797	26.068	18.517	−1.612
700	28.577	58.430	43.271	10.611	26.068	17.259	−1.288
800	29.434	62.299	45.412	13.510	26 068	16.000	−1.045
900	30.501	65.825	47.487	16.505	26.068	14.742	−0.856
1000	31.861	69.107	49.486	19.621	26.068	13.483	−0.704
1100	33.472	72.218	51.412	22.886	26.068	12.225	−0.581
1200	35.187	75.203	53.271	26.318	26 068	10.967	−0.477
1300	37.116	78.095	55.070	29.932	26.068	9.708	−0.390
1350.000	38.112	79.514	55.949	31.813	GLASS <– –> LIQUID		
1350.000	39.330	79.514	55.949	31.813	TRANSITION		
1400	39.330	80.944	56.816	33.779	26.103	8.449	−0.315
1500	39.330	83.658	58.516	37.712	26.020	7.190	−0.250
1600	39.330	86.196	60.168	41.645	25.727	5.943	−0.194
1700	39.330	88.581	61.770	45.578	25.219	4.720	−0.145
1800	39.330	90.829	63.322	49.511	24.492	3.535	−0.103
1900	39.330	92.955	64.827	53.444	23.542	2.395	−0.066
2000	39.330	94.972	66.284	57.377	22.368	1.311	−0.034
2100	39.330	96.891	67.696	61.310	20.967	0.292	−0.007
2130.000	39.330	97.449	68.111	62.490	– – – CRYSTAL <– –> LIQUID – – –		
2200	39.330	98.721	69.065	65.243	0.	0.	0.
2300	39.330	100.469	70.393	69.176	0.	0.	0.
2400	39.330	102.143	71.681	73.109	0.	0.	0.
2500	39.330	103.749	72.932	77.042	0.	0.	0.
2600	39.330	105.291	74.147	80.975	0.	0.	0.
2700	39.330	106.775	75.328	84.908	0.	0.	0.
2800	39.330	108.206	76.477	88.841	0.	0.	0.
2900	39.330	109.586	77.595	92.774	0.	0.	0.
2952.078	39.330	110.286	78.165	94.822	– – – – – FUGACITY = 1 bar – – – – –		
3000	39.330	110.919	78.684	96.707	−339.122	5.508	−0.096
3100	39.330	112.209	79.744	100.640	−338.294	16.982	−0.286
3200	39.330	113.457	80.779	104.572	−337.516	28.430	−0.464
3300	39.330	114.668	81.787	108.505	−336.786	39.855	−0.631
3400	39.330	115.842	82.772	112.438	−336.104	51.258	−0.787
3500	39.330	116.982	83.733	116.371	−335.469	62.641	−0.935

PREVIOUS: CURRENT: June 1973

Chromium (Cr)

CRYSTAL-LIQUID

0 to 2130 K crystal
above 2130 K liquid

Refer to the individual tables for details.

$A_r = 51.996$ Chromium (Cr) $Cr_1(cr,l)$

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

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−4.057	0.	0.	0.
100	9.963	4.286	41.746	−3.746	0.	0.	0.
200	19.860	14.869	25.680	−2.162	0.	0.	0.
250	22.298	19.590	23.998	−1.102	0.	0.	0.
298.15	23.434	23.618	23.618	0.	0	0.	0.
300	23.472	23.764	23.619	0.043	0.	0.	0.
311.500	23.681	24.651	23.641	0.315	____ C_p LAMBDA MAXIMUM ____		
311.500	23.681	24.654	23.641	0.316	TRANSITION		
350	24.393	27.453	23.908	1.240	0.	0.	0.
400	25.230	30.765	24.562	2.481	0.	0.	0.
450	25.983	33.781	25.421	3.762	0.	0.	0.
500	26.631	36.553	26.398	5.078	0.	0.	0.
600	27.719	41.508	28.513	7.797	0	0.	0.
700	28.577	45.846	30.686	10.612	0.	0.	0.
800	29.434	49.715	32.827	13.511	0.	0.	0.
900	30.501	53.241	34.902	16.505	0.	0.	0.
1000	31.861	56.523	36.901	19.621	0.	0.	0.
1100	33.472	59.634	38.828	22.887	0.	0.	0.
1200	35.187	62.618	40.687	26.318	0.	0.	0.
1300	37.116	65.511	42.485	29.933	0.	0.	0.
1400	39.125	68.334	44.231	33 744	0.	0	0.
1500	41.200	71.104	45.931	37.760	0.	0.	0.
1600	43.329	73.831	47.589	41.986	0.	0.	0.
1700	45.501	76.523	49.212	46.427	0.	0.	0.
1800	47.706	79.186	50.804	51.087	0.	0.	0.
1900	49 944	81.825	52.367	55.970	0.	0.	0
2000	52.204	84.444	53.905	61.077	0.	0.	0.
2100	54.488	87.046	55.422	66.411	0.	0.	0.
2130.000	55.174	87.824	55.873	68.056	____ CRYSTAL <--> LIQUID ____		
2130.000	39.330	97.449	55.873	88.558	TRANSITION		
2200	39.330	98.721	57.216	91.311	0.	0.	0.
2300	39.330	100.469	59.059	95.244	0.	0.	0.
2400	39.330	102.143	60.819	99.177	0.	0.	0.
2500	39.330	103.749	62.505	103.110	0.	0.	0.
2600	39.330	105.291	64.121	107.043	0.	0.	0.
2700	39.330	106.775	65.673	110.976	0.	0.	0.
2800	39.330	108.206	67.167	114.909	0.	0.	0.
2900	39.330	109.586	68.606	118.842	0.	0.	0
2952.078	39.330	110.286	69.335	120.890	----- FUGACITY = 1 bar -----		
3000	39.330	110.919	69.994	122.775	−339.122	5.508	−0.096
3100	39.330	112.209	71.335	126.708	−338.294	16.982	−0.286
3200	39.330	113.457	72.632	130.641	−337.516	28.430	−0 464
3300	39.330	114.668	73.888	134.574	−336.786	39.855	−0 631
3400	39.330	115.842	75.105	138.507	−336.104	51.258	−0 787
3500	39.330	116.982	76.285	142.440	−335.469	62.641	−0.935

PREVIOUS: CURRENT: June 1973

Chromium (Cr) $Cr_1(cr,l)$

Chromium (Cr) **IDEAL GAS** **$A_r = 51.996$ Chromium (Cr)** **$Cr_1(g)$**

IP(Cr, g) = 54570 ± 10 cm^{-1}
$S°(298.15\ K) = 174.31 \pm 0.4\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 395.34 \pm 4.2\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = 397.48 \pm 4.2\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ, cm^{-1}	g_i
$^7S_3$	0.00	7
$^5S_2$	7593.16	5
$^5D_0$	7750.78	1
$^5D_1$	7810.82	3
$^5D_2$	7927.47	5
$^5D_3$	8095.21	7
$^5D_4$	8307.57	9

Enthalpy of Formation

The many vapor pressure studies are treated by a 2nd and 3rd law analysis and are tabulated below. In all cases the reaction of interest is $Cr(cr) \rightarrow Cr(g)$.

Source	Data Points	T/K	Method	$\Delta_f H°(298.15\ K)$, kcal mol^{-1} 2nd law	3rd law	Drift $cal{\cdot}K^{-1}{\cdot}mol^{-1}$
1	15*	1283–1562	Langmuir	94.05 ± 0.84	94.82	0.54 ± 0.60
2	9	1162–1282	Knudsen	98.51 ± 2.16	95.28	−2.64 ± 1.77
3	10	1292–1509	Langmuir	97.60 ± 1.60	92.32	−3.71 ± 1.12
	10**	1187–1550		95 15 ± 1.00	91.82	−2.47 ± 0.74
4	9	1381–1505	Knudsen	101.14 ± 2.87	94.90	−4.29 ± 1.97
5	eqn	1502–1576	Knudsen	88.08	90.06	1.28
6	15	1317–1558	Knudsen	93.14 ± 5.70	93.99	0.59 ± 3.95
7	eqn	1441–1672	Knudsen	92.50	94.79	1.48
8	9	1273–1373	Knudsen	97.54 ± 2.93	95.97	−1.19 ± 2.23
9	eqn	1376–1592	Torsion–effusion	91.79	93.85	1.40
10	15**	1559–1805	Knudsen	92.78 ± 3.08	95.50	1.62 ± 1.84

* Two points neglected due to failure of a statistical test.
** One point neglected due to failure of a statistical test.

Early studies by Greenwood[11] and Baur and Brunner[12] are not considered as their work leads to $\Delta_f H°(298.15\ K)$ which are 10–15 $kcal{\cdot}mol^{-1}$ too low when compared to the results listed above.

We adopt $\Delta_f H°(298.15\ K) = 95.0 \pm 1.0\ kcal{\cdot}mol^{-1}$ for Cr(g). This value is representative of the more recent 2nd law values tabulated above.[7–10]

Heat Capacity and Entropy

The electronic levels and quantum weights are obtained from Moore;[13] although only the lowest levels are listed above. There are predicted levels which have not been observed and/or classified. It is anticipated that these levels will not significantly alter the entropy below 3000 K. The heat capacity and entropy values are very similar to those adopted bvy Hultgren *et al.*[14]

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

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_f H°$ (kJ·mol⁻¹)	$\Delta_f G°$ (kJ·mol⁻¹)	log K_f
0	0.	0.	INFINITE	−6.197	395.340	395.340	INFINITE
100	20.786	151.604	192.791	−4 119	397.107	382.375	−199.732
200	20.786	166.012	176.212	−2.040	397.602	367.374	−95.948
250	20.786	170.650	174.653	−1.001	397.581	359.816	−75.179
298.15	20.786	174.311	174.311	0.	397.480	352.551	−61.765
300	20.786	174.440	174.312	0.038	397.475	352.272	−61.336
350	20.786	177.644	174.565	1.078	397.317	344.750	−51.451
400	20.786	180.419	175.127	2.117	397.116	337.254	−44.041
450	20.786	182.868	175.854	3.156	396.874	329.785	−38.280
500	20.786	185.058	176 666	4.196	396.598	322.346	−33.675
600	20.786	188.847	178.390	6.274	395.957	307.554	−26.775
700	20.787	192.052	180.119	8.353	395.221	292.877	−21.855
800	20.790	194.828	181.788	10.432	394 401	278.311	−18.172
900	20.803	197.277	183.375	12.511	393.486	263.854	−15.314
1000	20.835	199.470	184.877	14.593	392.452	249.504	−13.033
1100	20.901	201.459	186.296	16.679	391.272	235.265	−11.172
1200	21.015	203.282	187.636	18.775	389.937	221.140	−9.626
1300	21 191	204.970	188.905	20.884	388.432	207.134	−8.323
1400	21 440	206.549	190.110	23.015	386.751	193.250	−7.210
1500	21.768	208.039	191.256	25.175	384.895	179.492	−6.250
1600	22.173	209.457	192.350	27.372	382.865	165.864	−5.415
1700	22.653	210.815	193.396	29.612	380.665	152.368	−4.682
1800	23.198	212.125	194.400	31.904	378.297	139.006	−4.034
1900	23.798	213.395	195.367	34.254	375.764	125.780	−3.458
2000	24.439	214.632	196.299	36.665	373.068	112.692	−2.943
2100	25.109	215.840	197.201	39.142	370.211	99.743	−2.481
2200	25.794	217.024	198.075	41.688	347.856	87.589	−2.080
2300	26.483	218.186	198.925	44.301	346.537	75.788	−1.721
2400	27.165	219.328	199.751	46.984	345.287	64.044	−1.394
2500	27.831	220.450	200.557	49.734	344.104	52.350	−1.094
2600	28.476	221.554	201.343	52.549	342.986	40.702	−0.818
2700	29.095	222.641	202.112	55.428	341.932	29.096	−0.563
2800	29.687	223.710	202.864	58.367	340.939	17.528	−0.327
2900	30.250	224 761	203.601	61.364	340.003	5.994	−0.108
2952.078	30.533	225.302	203.979	62.947	----- FUGACITY = 1 bar -----		
3000	30.788	225.796	204.324	64.417	0.	0.	0.
3100	31.302	226.814	205.033	67.521	0.	0.	0.
3200	31.796	227.815	205.729	70.676	0.	0.	0.
3300	32.275	228.801	206.413	73.880	0.	0.	0.
3400	32.745	229.772	207.086	77.131	0.	0.	0.
3500	33.212	230.728	207.748	80.429	0.	0.	0.
3600	33.680	231.670	208.399	83.773	0.	0.	0.
3700	34.156	232.599	209.041	87.165	0.	0.	0.
3800	34.646	233.516	209.673	90.605	0.	0.	0.
3900	35.157	234.423	210.296	94.095	0.	0.	0.
4000	35.692	235.320	210.910	97.637	0.	0.	0.
4100	36.260	236.208	211.517	101.235	0.	0.	0.
4200	36.864	237.089	212.115	104.890	0.	0.	0.
4300	37.511	237.964	212.706	108.609	0.	0.	0.
4400	38.205	238.834	213.290	112.394	0.	0.	0.
4500	38.954	239.701	213.867	116.252	0.	0.	0.
4600	39.760	240.566	214.438	120.187	0.	0.	0.
4700	40.632	241.430	215.003	124.206	0.	0.	0.
4800	41.572	242.295	215.563	128.315	0.	0.	0.
4900	42.587	243.163	216.117	132.523	0.	0.	0.
5000	43.681	244.034	216.667	136.835	0.	0.	0.
5100	43.917	244.834	217.207	140.898	0.	0.	0.
5200	44.964	245.697	217.746	145.342	0.	0.	0.
5300	46.064	246.564	218.282	149.892	0.	0.	0.
5400	47.221	247.435	218.814	154.556	0.	0.	0.
5500	48.432	248.313	219.342	159.338	0.	0.	0.
5600	49.697	249 197	219.867	164.244	0.	0.	0.
5700	51.009	250.087	220.390	169.277	0.	0.	0.
5800	52.370	250.986	220.909	174.445	0.	0.	0.
5900	53.779	251.893	221.427	179.752	0.	0.	0.
6000	55.230	252.809	221.942	185.202	0.	0.	0.

PREVIOUS: June 1979 (1 atm)   CURRENT. June 1979 (1 bar)

Chromium, Ion (Cr^+) IDEAL GAS $M_r = 51.99545$

$IP(Cr^+, g) = 133060 \pm 10\ cm^{-1}$
$S°(298.15\ K) = 173.029 \pm 0.05\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = 1048.14 \pm 1.5\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298\ 15\ K) = [1056.480]\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_n, cm^{-1}	g_i
$^6S_{5/2}$	0.00	6
$^6D_{1/2}$	1196.00	2
.	.	.
.	.	.
.	.	.
$^4G_{11/2}$	105421.9	12
IP	133060	

Enthalpy of Formation

$\Delta_f H°(Cr^+, g, 0\ K)$ is calculated from $\Delta_f H°(Cr, g, 0\ K)$[1] using the spectroscopic value of $IP(Cr) = 54570 \pm 10\ cm^{-1}$ ($652.80 \pm 0.12\ kJ{\cdot}mol^{-1}$) from Sugar and Corliss.[2] The ionization limit is converted from cm^{-1} to $kJ{\cdot}mol^{-1}$ using the factor, $1\ cm^{-1} = 0\ 01196266\ kJ{\cdot}mol^{-1}$, which is derived from the 1973 CODATA fundamental constants.[3] Rosenstock *et al.*[4] and Levin and Lias[5] have summarized additional ionization and appearance potential data.

$\Delta_f H°(Cr^+, g, 298.15\ K)$ is calculated from $\Delta_f H°(Cr, g, 0\ K)$ by using IP(Cr) with JANAF[1] enthalpies, $H°(0\ K)–H°(298.15\ K)$, for Cr(g), $Cr^+(g)$, and $e^-(ref)$. $\Delta_f H°(Cr \rightarrow Cr^+ + e^-, 298.15\ K)$ differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[4] $\Delta_f H°(298.15\ K)$ should be changed by $-6.197\ kJ\ mol^{-1}$ 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. Although we have listed only the ground, the first excited state, the highest observed excited state, and the ionization potential for $Cr^+(g)$, all levels listed by Sugar and Corliss,[2] as well as estimated levels, are used in the calculation. The observed levels are too numerous to list completely. The calculations indicate that for $Cr^+(g)$, the tehrmodynamic functions are independent of the estimated missing levels (for $n = 4$), the cut–off procedure, and the inclusion of $n = 6$ levels up to 6000 K, the Gibbs energy function showing variations of 0.02% at this temperature. The reported uncertainty is $S°(298.15\ K)$ is due to uncertainties in the relative ionic mass, and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states (n>6), and use of different fill and cut–off procedures.[6]

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Chromium, Ion (Cr^+) $Cr_1^+(g)$

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

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.197	1048.142		
100	20.786	150.322	191.510	−4.119			
200	20.786	164.730	174.931	−2.040			
250	20.786	169.368	173.372	−1.001			
298.15	20 786	173.029	173.029	0.	1056.480	1005.678	−176.191
300	20.786	173.158	173.030	0.038	1056.513	1005.363	−175.049
350	20.786	176.362	173.283	1.078	1057.395	996.767	−148.759
400	20.786	179.138	173.845	2.117	1058.232	988.049	−129.026
450	20.786	181.586	174.572	3.156	1059.030	979.227	−113.666
500	20.786	183.776	175.385	4.196	1059.793	970.319	−101.369
600	20.786	187.566	177.109	6.274	1061.231	952.288	−82.904
700	20.786	190.770	178.837	8.353	1062.573	934.023	−69.698
800	20.786	193.545	180.506	10.431	1063.832	915.572	−59.781
900	20.786	195.994	182.094	12.510	1064.995	896.968	−52.059
1000	20.786	198.184	183.595	14.589	1066.036	878.242	−45.875
1100	20.787	200.165	185.013	16.667	1066.927	859.418	−40.810
1200	20.790	201.974	186.352	18.746	1067.654	840.520	−36.587
1300	20.796	203.638	187.618	20.825	1068.197	821.569	−33.011
1400	20.808	205 180	188.818	22.906	1068.544	802.583	−29.945
1500	20.831	206.616	189.958	24.987	1068.689	783.580	−27.287
1600	20.868	207.961	191.041	27.072	1068.626	764.573	−24.961
1700	20.926	209.228	192.074	29.162	1068.353	745.577	−22.909
1800	21.008	210.426	193.061	31.258	1067.868	726.603	−21.085
1900	21.121	211.565	194.005	33.364	1067 170	707.662	−19.455
2000	21.269	212.652	194.910	35.484	1066.261	688.763	−17.989
2100	21.457	213.694	195.780	37.620	1065.141	669.915	−16.663
2200	21.686	214.698	196.617	39.776	1044.477	651.780	−15.475
2300	21.961	215.667	197.425	41.958	1044.805	633 923	−14.397
2400	22.283	216.609	198.204	44.170	1045.162	616.051	−13.408
2500	22.652	217.526	198.959	46.417	1045.554	598.164	−12.498
2600	23.069	218.422	199.690	48.702	1045.985	580.260	−11.658
2700	23.533	219.301	200.400	51.032	1046.461	562.338	−10.879
2800	24.044	220.166	201.091	53.410	1046.985	544.398	−10.156
2900	24.600	221.019	201.764	55.842	1047.562	526.439	−9.482
3000	25.199	221.863	202.419	58.332	709.076	513.967	−8.949
3100	25.839	222.700	203.060	60.883	710.601	507.438	−8.550
3200	26.517	223.531	203.687	63.501	712.142	500.860	−8.176
3300	27.230	224.358	204.301	66.188	713.704	494.233	−7.823
3400	27.975	225.182	204.903	68.948	715.292	487.559	−7.490
3500	28.750	226.004	205.494	71.784	716.908	480.837	−7.176
3600	29.550	226.825	206.075	74.699	718.557	474.069	−6.879
3700	30.374	227.646	206.647	77.695	720.240	467.255	−6.596
3800	31.218	228.467	207.210	80.774	721.958	460.394	−6.329
3900	32.078	229.289	207.766	83.939	723.712	453.488	−6.074
4000	32.952	230.112	208.314	87.190	725.499	446.537	−5.831
4100	33.838	230.936	208.856	90.530	727.320	439.540	−5.600
4200	34.733	231.763	209.392	93.958	729.171	432.499	−5.379
4300	35.635	232.590	209.921	97.477	731.050	425.413	−5.168
4400	36.542	233.420	210.446	101.085	732.952	418.283	−4.966
4500	37.452	234.251	210.966	104.785	734.873	411.110	−4.772
4600	38.366	235.085	211.481	108.576	736.807	403.894	−4.586
4700	39.282	235.920	211.992	112.458	738.749	396.636	−4.408
4800	40.199	236.756	212.499	116.432	740.692	389.336	−4.237
4900	41.118	237.594	213.003	120.498	742.629	381.996	−4.072
5000	42.040	238 434	213.503	124.656	744.553	374.617	−3.914
5100	42.964	239.276	214.000	128.906	746.819	367.172	−3.761
5200	43.893	240.119	214.494	133.249	748.797	359.709	−3.613
5300	44.827	240.964	214.986	137.685	750.761	352.208	−3.471
5400	45.767	241.811	215.475	142.215	752.705	344.669	−3.334
5500	46.716	242.659	215.961	146.839	754.626	337.095	−3.201
5600	47.675	243.510	216.446	151.558	756.518	329.487	−3.073
5700	48.645	244.362	216.928	156.374	758.379	321.845	−2.949
5800	49.629	245.217	217.408	161.288	760.204	314.170	−2.829
5900	50 627	246.073	217.887	166.300	761.988	306.464	−2.713
6000	51.640	246 933	218.364	171.414	763.730	298 729	−2.601

PREVIOUS: CURRENT. March 1984 (1 bar)

Chromium, Ion (Cr^+) $Cr_1^+(g)$

Chromium, Ion (Cr^-) IDEAL GAS $M_r = 51.99655$ Chromium, Ion (Cr^-) $Cr_1^-(g)$

EA(Cr, g) = 0.666 ± 0.012 eV
S°(298.15 K) = 173.030 ± 0.003 $J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H^\circ$(0 K) = 331.081 ± 2 $kJ \cdot mol^{-1}$
$\Delta_f H^\circ$(298.15 K) = [327.024] $kJ \cdot mol^{-1}$

Electonic Level and Quantum Weight		
State	ϵ_i, cm^{-1}	g_i
$^6S_{5/2}$	0.0	6

Enthalpy of Formation

$\Delta_f H^\circ(Cr^-, g, 0\ K)$ is calculated from $\Delta_f H^\circ(Cr, g, 0\ K)$[1] using the adopted electron affinity of EA(Cr) = 0.666 ± 0 012 eV (64.259 ± 1.158 $kJ \cdot mol^{-1}$). This value, recommended by Hotop and Lineberger[2] is based on a laser photodetachment electron spectrometry study.[3] Additional information on $Cr^-(g)$ may be obtained in the critical discussions of Hotop and Lineberger,[2, 4] Rosenstock *et al.*[5] and Massey.[6]

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

Heat Capacity of Entropy

The ground state electronic configuration for $Cr^-(g)$ is given by Hotop and Lineberger[2, 4] and Rosenstock *et al.*[5] Lacking any experimental evidence as to the stability of any excited states, we assume that no stable excited states exist.

References

[1] JANAF Thermochemical Tables: Cr(g), 6–30–73; e^-(ref), 3–31–82.
[2] H. Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data, 14, 731 (1985).
[3] C. S. Feigerle, R. P. Corderman, S. V. Bobashev and W. C. Lineberger, J. Chem. Phys. 74, 1580 (1981).
[4] H. Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data 4, 539 (1975).
[5] H. M. Rosenstock, K. Draxl *et al.*, J. Phys. Chem. Ref. Data 6, Supp. 1 (1977).
[6] H. S. W. Massey, "Negative Ions," 3rd ed., Cambridge University Press, Cambridge, (1976).

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

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−6.197	331.081		
100	20.786	150.322	191.510	−4.119			
200	20.786	164.730	174.931	−2.040			
250	20.786	169.368	173.372	−1.001			
298.15	20.786	173.030	173.030	0.	327.024	288.732	−50.585
300	20.786	173.158	173.030	0.038	326.981	288.494	−50.231
350	20.786	176.362	173.283	1.078	325.783	282.174	−42.112
400	20.786	179.138	173.845	2.117	324.543	276.028	−36.046
450	20.786	181.586	174.572	3.156	323.262	270.041	−31.345
500	20.786	183.776	175.385	4.196	321.946	264.197	−27.601
600	20.786	187.566	177.109	6.274	319.227	252.901	−22.017
700	20.786	190.770	178.837	8.353	316.412	242.068	−18.063
800	20.786	193.546	180.506	10.431	313.513	231.644	−15.125
900	20.786	195.994	182.094	12.510	310.519	221.590	−12.861
1000	20.786	198.184	183.595	14.589	307.403	211.874	−11.067
1100	20.786	200.165	185.013	16.667	304.137	202.478	−9.615
1200	20.786	201.974	186.352	18.746	300.706	193.387	−8.418
1300	20.786	203.637	187.619	20.824	297.091	184.589	−7.417
1400	20.786	205.178	188.819	22.903	293.280	176.076	−6.569
1500	20.786	206.612	189.958	24.982	289.264	167.844	−5.845
1600	20.786	207.953	191.041	27.060	285.038	159.886	−5.220
1700	20.786	209.214	192.073	29.139	280.597	152.198	−4.676
1800	20.786	210.402	193.059	31.217	275.937	144.779	−4.201
1900	20.786	211.526	194.001	33.296	271.054	137.625	−3.784
2000	20.786	212.592	194.904	35.375	265.947	130.733	−3.414
2100	20.786	213.606	195.771	37.453	260.612	124.103	−3.087
2200	20.786	214.573	196.604	39.532	235.713	118.387	−2.811
2300	20.786	215.497	197.405	41.610	231.780	113.142	−2.570
2400	20.786	216.381	198.178	43.689	227.847	108.068	−2.352
2500	20.786	217.230	198.923	45.768	223.914	103.158	−2.155
2600	20.786	218.045	199.643	47.846	219.981	98.405	−1.977
2700	20.786	218.830	200.339	49.925	216.048	93.804	−1.815
2800	20.786	219.586	201.013	52.004	212.115	89.348	−1.667
2900	20.786	220.315	201.666	54.082	208.182	85.033	−1.532
3000	20.786	221.020	202.299	56.161	−134.873	86.362	−1.504
3100	20.786	221.701	202.914	58.239	−137.977	93.788	−1.580
3200	20.786	222.361	203.512	60.318	−141.132	101.314	−1.654
3300	20.786	223.001	204.093	62.397	−144.336	108.940	−1.724
3400	20.786	223.621	204.658	64.475	−147.587	116.664	−1.792
3500	20.786	224.224	205.209	66.554	−150.885	124.484	−1.858
3600	20.786	224.809	205.745	68.632	−154.229	132.399	−1.921
3700	20.786	225.379	206.268	70.711	−157.621	140.407	−1.982
3800	20.786	225.933	206.778	72.790	−161.061	148.508	−2.041
3900	20.786	226.473	207.276	74.868	−164.551	156.700	−2.099
4000	20.786	226.999	207.763	76.947	−168.093	164.982	−2.154
4100	20.786	227.513	208.238	79.025	−171.691	173.353	−2.209
4200	20.786	228.014	208.703	81.104	−175.347	181.813	−2.261
4300	20.786	228.503	209.158	83.183	−179.065	190.361	−2.312
4400	20.786	228.981	209.603	85.261	−182.850	198.996	−2.362
4500	20.786	229.448	210.039	87.340	−186.708	207.717	−2.411
4600	20.786	229.905	210.466	89.418	−190.643	216.526	−2.459
4700	20.786	230.352	210.884	91.497	−194.662	225.420	−2.505
4800	20.786	230.789	211.294	93.576	−198.771	234.401	−2.551
4900	20.786	231.218	211.697	95.654	−202.979	243.469	−2.595
5000	20.786	231.638	212.091	97.733	−207.291	252.624	−2.639
5100	20.786	232.049	212.479	99.811	−211.354	261.839	−2.682
5200	20.786	232.453	212.859	101.890	−215.798	271.160	−2.724
5300	20.786	232.849	213.232	103.969	−220.348	280.568	−2.765
5400	20.786	233.237	213.599	106.047	−225.012	290.063	−2.806
5500	20.786	233.619	213.960	108.126	−229.794	299.645	−2.846
5600	20.786	233.993	214.314	110.204	−234.700	309.315	−2.885
5700	20.786	234.361	214.663	112.283	−239.733	319.074	−2.924
5800	20.786	234.723	215.005	114.362	−244.901	328.923	−2.962
5900	20.786	235.078	215.343	116.440	−250.208	338.862	−3.000
6000	20.786	235.428	215.674	118.519	−255.658	348.891	−3.037

PREVIOUS: CURRENT: March 1984 (1 bar)

Chromium, Ion (Cr^-) $Cr_1^-(g)$

Chromium Nitride (CrN) CRYSTAL $M_r = 66.0027$

$S°(298.15\ K) = 37.71 \pm 2.1\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -116.46 \pm 8.4\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -117.15 \pm 8.4\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

2nd and 3rd law analyses of equilibrium nitrogen pressures for the reaction $Cr_2N(cr) + 0.5\ N_2(g) = 2\ CrN(cr)$ cited in a recent review[1] of the thermodynamic properties of the Cr–N system are made using revised thermal functions for Cr_2N [2] and CrN (refer below) We have not taken into account, in our analysis, any variations in the compositions of the two nitrides (see Phase Data Section). Results of our analysis are tabulated below.

Source	Data Points	T/K	$\Delta_r H°$, kcal mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°(298.15\ K)^a$ kcal·mol^{-1}
Valensi[3]	8	1083–1288	−25.9	24.88 ± 0.37	0.8 ± 1.0	−27.4 ± 1.7
Sano[4]	6	1104–1223	−28.5	26.58 ± 0.16	1.7 ± 0.3	−28.3 ± 1.1
Smith[5]	10[b]	1178–1351	−13.0	25.0 ± 1.2	−9.5	−27.5 ± 1.6
Mills[6]	Equation	1173–1323	−25.1	25.26 ± 0.02	−0.2	−27.6 ± 1.0

[a] Third law values; auxiliary data used $\Delta_f H°(Cr_2N, cr, 298.15\ K) = -30.0 \pm 3.0\ kcal{\cdot}mol^{-1}$.
[b] Data taken from reference[1], one point rejected due to failure of a statistical test.

The equilibrium pressures of Sano[4] are inconsistent with those of the other investigations, and no weight is given to these results. Reasons for these discrepancies have been presented by DeLuca and Leitnaker.[1] The drifts are both positive and negative which provides support for our revised thermal functions for the two nitrides. Neumann *et al.*[7] measured $\Delta_f H°$ directly by combination of the elements in a bomb calorimeter. Two samples of chromium (99.2–99.7% purity) were heated to temperatures near 1200 K in 25 atmospheres of nitrogen. Under these conditions,[8] it is unlikely that significant amounts of subnitride (Cr_2N) were formed. Neumann *et al.*[7] recommended the value $\Delta_f H°(CrN, cr, 298.15\ K) = -29.5 \pm 0.5\ kcal{\cdot}mol^{-1}$.

We adopt $\Delta_f H°(CrN, cr, 298.15\ K)$ value of $-28.0 \pm 2.0\ kcal{\cdot}mol^{-1}$ ($-117.152 \pm 8.4\ kJ{\cdot}mol^{-1}$) which is based mainly on the results from two equilibrium studies[3,6] and to a lesser extent on the value determined by bomb calorimetry. Our adopted value agrees with that (−28.4 ± 1.5) selected by DeLuca and Leitnaker[1] but is 1.8 kcal·mol^{-1} less negative than the NBS[9] value (−29.8).

Heat Capacity and Entropy

One low temperature heat capacity study[10] has been reported for CrN which covered the temperature range 73–315 K. $C_p°$ values taken from the graph at 25° temperature intervals are used to obtain a value for $S°(298.15\ K)$ by integration. This method leads to $S°(298.15\ K) = 9.0$ cal K^{-1}·mol^{-1} (37.656 J·K^{-1}·mol^{-1}) with $S°(73\ K) = 0.39$ cal K^{-1}·mol^{-1}. The latter value is obtained from the Debye function D(530/T). The uncertainty in our value for $S°(298.15\ K)$ is believed to be less than ±0.5 cal·K^{-1}·mol^{-1}. Previously published estimates of $S°(298.15\ K)$ are 8.56[1] and 7.85.[11] The low temperature data set[10] contains a lambda peak at 281.7 K with $C_p°$ near the maximum equal to 75.1 cal·K^{-1}·mol^{-1}. Other transition temperatures have been reported as 286 K[12] and 287 K.[13] The anomaly arises from an antiferromagnetic–paramagnetic transformation[12,13] which is accompanied by an orthorhombic to cubic structural change.[14]

Satoh[15] has measured the heat contents of three chromium nitride samples at three temperatures each (372.6, 598.8, and 784.2 K), in an ice calorimeter. DeLuca and Leitnaker[1] have reevaluated his heat contents and presented $C_p°$ data for CrN in the temperature range 298–1400 K. Their values above 400 K are adopted and joined smoothly with the low temperature $C_p°$ data[10] near 350 K. $C_p°$ data above 1400 K are obtained by graphical extrapolation.

Phase Data

The homogeneity range of the CrN phase is not known; however, results of two recent studies[6,12] indicate that it is probably much smaller than that for Cr_2N.[2] X-ray diffraction patterns[16,17] for CrN have been interpreted in terms of a cubic structure (NaCl type). Other information on the chromium–chromium nitride system has been reviewed by Storms.[8]

Decomposition Data

No information is available on the melting point of CrN. Upon heating we assume that the compound decomposes to its elements rather than melting. T_{dcm} is the temperature at which $\Delta_f G°$ for the process $CrN(cr) = Cr(cr) + 0.5\ N_2(g)$ equals zero.

References

[1] J. P. DeLuca and J. M. Leitnaker, J. Amer. Chem. Soc. 56, 126 (1973).
[2] JANAF Thermochemical Table. $Cr_2N(cr)$, 12–31–73.
[3] G. Valenski, J Chim. Phys. Physicochim. Biol. 26, 202 (1929).
[4] K Sano, Nippon Kagaku Kaishi 58, 981 (1937).
[5] W. H. Smith, Ph.D. Thesis, Rensselaer Polytechnic Institute, Troy, N. Y., (1958).
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Continued on page 975

Chromium Nitride (CrN) $Cr_1N_1(cr)$

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

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−7.705	−116.465	−116.465	INFINITE
100	9.985	3.850	78.059	−7.421	−117.943	−109.909	57.410
200	29.126	16.556	43.947	−5.478	−119.039	−101.378	26.477
298.15	52.677	37.711	37.711	0.	−117.152	−92.790	16.256
300	51.393	38.033	37.712	0.096	−117.126	−92.639	16.130
400	49.078	51 780	39.599	4.873	−116.350	−84.587	11.046
500	49.748	62.804	43.176	9.814	−115.475	−76.749	8.018
600	50.417	71.933	47.229	14.822	−114.678	−69.080	6.014
700	51.087	79.756	51.330	19.898	−113.938	−61.539	4.592
800	51.714	86.618	55.321	25.037	−113.252	−54.101	3.532
900	52.384	92.748	59.145	30.242	−112.630	−46.745	2.713
1000	53.053	98.301	62.787	35.514	−112.094	−39.455	2.061
1100	53.723	103.389	66.250	40.853	−111.670	−32.212	1.530
1200	54.392	108.093	69.544	46.259	−111.369	−25.003	1.088
1300	55.020	112.471	72.679	51.729	−111.211	−17.813	0.716
1400	55.689	116.573	75.669	57.264	−111.204	−10.630	0.397
1500	56.379	120.439	78.526	62.868	−111.350	−3 442	0.120
1600	57.028	124.098	81.261	68.538	−111.655	3.761	−0.123
1700	57.697	127.575	83.884	74.275	−112.123	10.988	−0.338
1800	58.367	130.892	86.404	80.078	−112.755	18.247	−0.530
1900	59.078	134.066	88.830	85.949	−113.550	25.546	−0.702
2000	59.831	137.117	91.168	91.897	−114.504	32.891	−0.859
2100	60.375	140.049	93.427	97.906	−115.632	40.287	−1.002
2200	61.003	142.872	95.610	103.974	−136.273	48.397	−1.149
2300	61.714	145.599	97.725	110.110	−135.887	56.783	−1.290
2400	62.467	148.242	99.775	116.320	−135.433	65.150	−1.418
2500	63.074	150.805	101.765	122.598	−134.915	73.497	−1.536

PREVIOUS: CURRENT December 1973

$S°(298.15\ K) = 230.553 \pm 8.4\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_fH°(0\ K) = 504.62 \pm 20.9\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = 505.01 \pm 20.9\ kJ{\cdot}mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i, cm^{-1}	g_i
$^4\Sigma$	0	[4]
	[15000]	[8]
	[20000]	[4]

ω_e = [1000] cm^{-1} ω_ex_e = [5.0] cm^{-1} σ = 1
B_e = [0.56115] cm^{-1} α_e = [0.00375] cm^{-1} r_e = [1.65] Å

Enthalpy of Formation

Srivastava and Farber[1] have observed mass spectrometrically CrN(g) as one of the vapor species in equilibrium with the Cr–V–N system. A substitution reaction between VN and Cr was employed in the formation of gaseous mononitride in the temperature range 1900 to 2063 K. Ion intensities for the equilibrium species CrN, VN, V, and N_2 were measured and converted to partial pressures by means of an intensity-pressure relationship for Au(g). Results of a 2nd and 3rd law analysis of their pressure data[1] are given below.

Reaction	Data Points	T/K	$\Delta_rH°$(298.15 K), kcal·mol^{-1} 2nd Law	3rd Law	Drift cal·K^{-1}·mol^{-1}	$\Delta_fH°$(298.15 K)^a, kcal·mol^{-1} 2nd Law	3rd Law
A	7	1903–2063	−35.6	−27.18 ± 0.75	4.3 ± 2.3	130.6	122.2
B	7	1903–2063	21.3	22 42 ± 0.33	0.6 ± 1.3	118.1	119.2

Reactions: (A) CrN(g) = Cr(g) + 0.5 N_2(g) (B) VN(g) + Cr(g) = CrN(g) + V(g)
^{a}Auxiliary $\Delta_fH°$ data[2] used (in kcal·mol^{-1}): Cr(g), 95.0 ± 1.0; VN(g), 125 ± 5; V(g), 123.2 ± 2.0.

We note that several of the log K_p values listed by Srivastava and Farber[1] for the two gas phase reactions are inconsistent with their reported partial pressure data. Since the 3rd law method is relatively insensitive to errors in the equilibrium constant, we believe the two 3rd law $\Delta_fH°$ values are more reliable than those obtained by the 2nd law. Thus, we adopt the average 3rd law value of $\Delta_fH°$(CrN, g, 298 15 K) = 120.7 ± 5.0 kcal·mol^{-1} (505.009 ± 20.9 kJ·mol^{-1}). Taking into account estimated errors in the pressure determinations and thermal functions, an overall uncertainty of ±5 kcal·mol^{-1} is assigned. The adopted $\Delta_fH°$ value corresponds to a dissociation energy of $\Delta_aH°$(CrN, g, 298.15 K) = 87.3 kcal·mol^{-1}.

Although no other experimental value for $\Delta_aH°$ is available, two estimations have been reported. Gingerich,[4] using empirical correlations of Colin and Goldfinger[3] and Pauling,[6] predicted a value of $\Delta_aH°$(CrN, g, 298.15 K) = 96 kcal·mol^{-1} for CrN(g) by both methods. This predicted value is in reasonable agreement with that determined experimentally by Srivastava and Farber[1] and reaffirms the usefulness of three empirical correlations[3-5] in predicting dissociation energies for gaseous diatomic mononitrides.

Heat Capacity and Entropy

The value of r_e(CrN) is obtained from the expression $r_e(MO) - r_e(MN) = -0.023$ Å with r_e(CrO) = 1.627 Å.[2] Differences in the bond lengths[7] for the oxides and nitrides of As, B, P, Si, and Ti are used to establish the value of −0.023. B_e is calculated from the estimated value for r_e. The moment of inertia is calculated to be 4.9881 × 10^{-39} g cm^2. The value of α_e is obtained from the other constants assuming a Morse potential function. The values of ω_e and ω_ex_e are assumed to lie between those for VO[2] and AsN.[7]

CrN is isoelectronic with VO; therefore, the ground state electronic configuration is taken to be the same as that for VO[2]. Also, the electronic levels and quantum weights are estimated by analogy with those for VO.[2] Futher support for the quartet ground state of CrN is provided by the fact that the atomic levels for Cr^{+3}[8] are also quartets. Our adopted upper levels and quantum weights contribute 0.13 cal·K^{-1}·mol^{-1} to the entropy of CrN at 4000 K.

References

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

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	$C_p°$	S°	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0	0.	0.	INFINITE	−8.778	504.624	504.624	INFINITE
100	29.107	198.342	257.038	−5.870	505.769	494.354	−258.224
200	29.454	218.573	233.318	−2.949	505.651	482.908	−126.123
250	30.032	225.203	231.055	−1.463	505.349	477.256	−99.717
298.15	30.754	230.553	230.553	0.	505.009	471.876	−82.671
300	30.783	230.743	230.553	0.057	504.995	471.670	−82.125
350	31.576	235.548	230.931	1.616	504.525	466.157	−69.570
400	32.327	239.814	231.779	3.214	504.152	460.702	−60.161
450	33.000	243.661	232.889	4.847	503.772	455.293	−52.849
500	33.586	247.169	234.145	6.512	503.384	449.927	−47.004
600	34.517	253.379	236.846	9.920	502.581	439.311	−38.245
700	35.197	258.754	239.601	13.407	501.732	428.832	−32.000
800	35.698	263.488	242.297	16.953	500.824	418.479	−27.324
900	36.077	267.716	244 890	20.543	499.831	408.245	−23.694
1000	36.369	271.533	247.367	24.166	498.718	398.127	−20.796
1100	36.599	275.010	249.724	27.815	497.453	388.127	−18.431
1200	36.786	278.203	251.966	31.484	496.017	378.251	−16.465
1300	36.939	281.154	254.099	35.171	494.392	368.502	−14.807
1400	37.069	283.896	256.131	38.871	492.564	358.885	−13.390
1500	37.180	286.457	258.068	42.584	490.527	349.406	−12.167
1600	37.277	288.860	259.918	46.307	488.274	340.070	−11.102
1700	37.365	291.123	261.688	50.039	485.802	330.882	−10 167
1800	37.447	293.261	263.383	53.780	483.108	321.846	−9.340
1900	37.525	295.287	265.009	57.528	480.189	312.966	−8.604
2000	37.601	297.214	266.572	61.284	477.044	304.245	−7.946
2100	37 679	299.051	268.075	65.048	473.671	295.687	−7.355
2200	37.760	300.805	269.523	68.820	450.734	287.950	−6.837
2300	37.846	302.486	270.920	72.601	448.764	280.595	−6.373
2400	37 938	304.098	272.269	76.390	446.798	273.325	−5.949
2500	38.039	305.649	273.574	80.188	444.835	266.137	−5.561
2600	38.149	307.143	274.836	83.998	442.878	259.028	−5.204
2700	38.269	308.585	276.059	87.819	440.928	251.994	−4.875
2800	38.400	309.979	277.246	91.652	438.987	245.032	−4.571
2900	38.542	311.329	278.398	95.499	437.055	238.139	−4.289
3000	38.695	312.638	279.518	99.361	96.116	235.926	−4.108
3100	38.860	313.910	280.607	103.238	95.036	240.604	−4.054
3200	39.037	315.146	281.667	107.133	93.919	245.317	−4.004
3300	39.224	316.350	282.700	111.046	92.769	250.066	−3.958
3400	39.422	317.524	283.707	114.978	91.588	254.850	−3.915
3500	39.629	318.670	284.690	118.931	90.378	259 670	−3.875
3600	39.846	319.789	285.649	122.904	89.139	264.524	−3.838
3700	40.071	320.884	286.587	126.900	87.874	269.413	−3.803
3800	40.303	321.956	287.503	130.919	86.580	274.337	−3.771
3900	40.541	323.006	288.400	134.961	85.258	279.295	−3.741
4000	40.785	324.035	289.278	139.027	83.905	284.288	−3.712
4100	41.034	325.045	290.138	143.118	82.521	289.314	−3.686
4200	41.286	326.037	290.981	147.234	81.100	294.375	−3.661
4300	41.541	327.012	291.808	151.376	79.641	299.470	−3.638
4400	41.797	327.969	292.619	155.542	78.138	304.600	−3.616
4500	42.054	328.912	293.415	159.735	76.587	309.764	−3.596
4600	42.310	329.839	294.197	163.953	74.982	314.963	−3.577
4700	42.565	330.751	294.965	168.197	73.318	320.198	−3.559
4800	42.819	331.650	295.720	172.466	71.586	325.469	−3.542
4900	43.069	332.536	296.462	176.761	69.780	330.777	−3.526
5000	43.316	333.408	297.192	181.080	67.892	336.122	−3.511
5100	43.559	334.268	297.911	185.424	66.276	341.479	−3.497
5200	43.797	335.117	298.618	189.792	64.302	346.895	−3.485
5300	44.030	335.953	299.315	194.183	62.244	352.349	−3.473
5400	44.257	336.778	300.001	198.597	60.093	357.842	−3.461
5500	44.478	337.592	300.677	203.034	57.844	363.377	−3.451
5600	44.693	338.396	301.343	207.493	55.492	368.953	−3.441
5700	44.900	339.189	302.000	211.973	53.032	374.572	−3.433
5800	45.101	339.971	302.648	216.473	50.456	380.235	−3.424
5900	45.293	340.744	303.288	220.992	47.758	385.944	−3.417
6000	45.479	341.507	303.918	225.531	44.934	391.700	−3.410

PREVIOUS: December 1973 (1 atm) CURRENT: December 1973 (1 bar)

Chromium Oxide (CrO) **IDEAL GAS** **$M_r = 67.9954$** **Chromium Oxide (CrO)** **$Cr_1O_1(g)$**

$S°(298.15\ K) = 239.268 \pm 6.3\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 187.85 \pm 41.8\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 188.28 \pm 41.8\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ_i cm^{-1}	g_i
X^5	0	10
B^5	16584.5	10

$\omega_e = 898.8$ cm–1
$B_e = 0.5286\ cm^{-1}$
$\omega_e x_e = 6.50\ cm^{-1}$
$\alpha_e = 0.0050\ cm^{-1}$
$\sigma = 1$
$r_e = 1.627$ Å

Enthalpy of Formation

Based on the adopted ground state vibrational constants, a linear Birge–Sponer extrapolation yields a dissociation energy, of 3.796 eV (87.54 kcal·mol^{-1}). Applying a correction for the ionicity in the Cr–O bond,[1] we recalculate $D_0^\circ = 4.017$ eV (92.63 kcal·mol^{-1}). This in turn corresponds to $\Delta_f H°(298.15\ K) = 60.95$ kcal·mol^{-1} for CrO(g), using auxiliary data.[2]

Huldt and Lagerqvist,[3] using a spectroscopic flame technique, reported $D_0^\circ = 4.4 \pm 0.5$ eV for CrO(g). This value was later corrected to $D_0^\circ = 5.3$ eV (122.9 kcal·mol^{-1}).[4,5] Grimley *et al.*[6] mentioned that in determining D_0° values by the flame technique of Huldt and Lagerqvist,[3] the calculation assumes that Cr and CrO are the only gaseous species containing Cr and that the $CrO_2(g)$ partial pressure cannot be neglected under these experimental conditions.

Grimley *et al.*[6] studied the vaporization of $Cr_2O_3(cr)$ under neutral and oxidizing conditions using mass spectrometric methods. The reported partial pressure data for Cr(g), CrO(g), $CrO_2(g)$, O(g), and $O_2(g)$ may be analyzed in terms of many different chemical equilibria. Our analyses of four equilibria in the neutral and oxidizing conditions are tabulated below.

	Reaction	$\Delta_r H°(298.15\ K)$, kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_f H°(298.15\ K)$, kcal·mol^{-1} 2nd law	3rd law
Neutral conditions	A*	−39.5	−44.9	−2.8 ± 2.1	55.5	50.1
1842–2062 K	B	−108.2	−100.4	4.0 ± 1.4	46.3	54.2
13 points	C	174.0	178.2	2.1 ± 1.2	38.4	42.6
	D*	206.3	205.9	−0.2 ± 1.4	40.9	40.5
Oxidizing conditions	A	−27.2	−43.7	−8.6 ± 13.1	67.8	51.3
1893–1945 K	B	−46.9	−99.3	−27.3 ± 4.0	107.6	55.2
3 points	C	192.2	181.0	−5 8 ± 4.4	56.6	45.4
	D	202.0	208.9	3.6 ± 9.0	36.6	43.5

Reaction A: $Cr(g) + 1/2\ O_2(g) = CrO(g)$ C: $1/2\ Cr_2O_3(cr) = CrO(g) + 1/4\ O_2(g)$
B: $Cr(g) + O(g) = CrO(g)$ D: $1/2\ Cr_2O_3(cr) = CrO(g) + 1/2\ O(g)$
*One point rejected due to a statistical test (1842 K).

The drifts are less severe in the netural system so that there is better agreement in the 2nd and 3rd law results for the neutral conditions than in the oxidizing system. Note that the 3rd law $\Delta_f H°(298.15\ K)$ values are slightly more positive for the oxidizing than the netural conditions for corresponding equilibria. The calculated $\Delta_f H°(298.15\ K)$ values for the gas phase (reactions A and B) are about 10 kcal·mol^{-1} higher than those of the condensed phase (reactions C and D) equilibria. Grimley *et al.*[6] prefer the gas phase results while Brewer and Rosenblatt[7] prefer the condensed phase results. We adopt $\Delta_f H°(CrO,\ cr,\ 298.15\ K) = 45.0 \pm 10.0$ kcal·mol^{-1} (188.280 ± 41.8 kJ·mol^{-1}) as a value which is representative of the 2nd and 3rd law results in the neutral system. The adopted $\Delta_f H°$ value leads to $D° = 4.71$ eV (108.6 kcal·mol^{-1}).

Chizhikov *et al.*[8] also studied the vaporization of Cr_2O_3 via mass spectrometry in the range 1690–2020 K. They reported the detection of gaseous Cr, CrO, CrO_2, and O during the evaporation process. The reported smoothed partial pressures of CrO(g) and $CrO_2(g)$ lie higher than those reported by Grimley *et al.*[6] by a factor of 2–5, while the partial pressures of Cr(g) are less than a factor 2 different. These data were not analyzed.

Heat Capacity and Entropy

The spectroscopic work involving CrO(g) has been reviewed and referenced by Rosen.[9] The adopted vibration and rotation constants as well as the electronic levels are those tabulated by Rosen.[9] The ground state has not been firmly established. Weltner[10] suggested a possible $^3\Sigma^-$ ground state. The free energy functions used here are 1.02 cal·K^{-1}·mol^{-1} at 298 K and 1.57 cal·K^{-1}·mol^{-1} at 3000 K lower than those suggested by Brewer and Rosenblatt.[7] The difference arises in that Brewer and Rosenblatt[7] approximated the CrO electronic levels with Cr^{++} electronic levels. The latter has a singlet ground state and many levels lying below 600 cm^{-1}.

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

	J·K^{-1}mol^{-1}			kJ·mol^{-1}			
T/K	C_p°	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−8.828	187.851	187.851	INFINITE
100	29.111	206.841	266.039	−5.920	188.996	177.405	−92.667
200	29.697	227.123	242.076	−2.991	188.885	165.783	−43.298
250	30.467	233.829	239.778	−1.487	188.599	160.039	−33.438
298.15	31.320	239.268	239.268	0.	188.280	154.567	−27.079
300	31.353	239.461	239.268	0.058	188.267	154.357	−26.876
350	32.214	244.360	239.653	1.647	187.818	148.746	−22.199
400	32.982	248.713	240.518	3.278	187.460	143.188	−18.698
450	33.643	252.637	241.650	4 944	187.087	137.677	−15.981
500	34.201	256.211	242.930	6.640	186.697	132.207	−13.812
600	35.062	262.527	245.684	10.106	185.863	121.387	−10.568
700	35.676	267.981	248.489	13.645	184.959	110.711	−8.261
800	36.125	272.776	251.231	17.236	183.983	100.170	−6.540
900	36.463	277.051	253.867	20.866	182.916	89.756	−5.209
1000	36.725	280.907	256.381	24.526	181.729	79.467	−4.151
1100	36.934	284.417	258.773	28.209	180.392	69.305	−3.291
1200	37.106	287.638	261.046	31.911	178.889	59.271	−2.580
1300	37.250	290.614	263.207	35.629	177.201	49.370	−1.984
1400	37.373	293.379	265.265	39.361	175.314	39.606	−1.478
1500	37.481	295.962	267.226	43.103	173.220	29.984	−1.044
1600	37.576	298.384	269.098	46.856	170.914	20.509	−0.670
1700	37 663	300 664	270.889	50.618	168.388	11.185	−0.344
1800	37.742	302.819	272.603	54.389	165.641	2.016	−0.059
1900	37.816	304.862	274.248	58.167	162.667	−6.994	0.192
2000	37.887	306.803	275.828	61.952	159.463	−15.842	0.414
2100	37.955	308.654	277.347	65.744	156.028	−24.523	0.610
2200	38.021	310.421	278.811	69.543	133.023	−32.381	0.769
2300	38 087	312.112	280.222	73.348	130.980	−39.854	0.905
2400	38.153	313 735	281.585	77.160	128.933	−47.237	1.028
2500	38.220	315.294	282.902	80.979	126.881	−54.536	1.139
2600	38.289	316.794	284 177	84.804	124.825	−61.752	1.241
2700	38.361	318.240	285.412	88.637	122.766	−68.889	1.333
2800	38.435	319.637	286.609	92.476	120.704	−75.949	1.417
2900	38.512	320.987	287.772	96.324	118.640	−82.936	1.494
3000	38.593	322.294	288.901	100.179	−222.444	−85.239	1.484
3100	38.677	323.561	289.999	104.042	−223.683	−80.645	1.359
3200	38.765	324.790	291.067	107.914	−224.973	−76.011	1.241
3300	38.856	325.984	292.107	111.795	−226.311	−71.335	1.129
3400	38.952	327.146	293.120	115.686	−227.696	−66.618	1.023
3500	39.050	328.276	294.109	119.586	−229.126	−61.860	0.923
3600	39.153	329.378	295.073	123.496	−230.600	−57.060	0.828
3700	39.258	330.452	296.015	127.416	−232.118	−52.219	0.737
3800	39.367	331.500	296.935	131.348	−233.681	−47.336	0.651
3900	39.478	332.524	297.834	135.290	−235.290	−42.411	0.568
4000	39.592	333.525	298.714	139.243	−236.946	−37.444	0.489
4100	39.709	334.504	299.575	143.208	−238.653	−32.436	0.413
4200	39.827	335.462	300.418	147.185	−240.413	−27.385	0.341
4300	39.947	336.401	301.244	151.174	−242.229	−22.291	0.271
4400	40.069	337.321	302.054	155.175	−244 107	−17.155	0.204
4500	40.191	338.223	302.848	159.188	−246.050	−11.976	0.139
4600	40.315	339.107	303.626	163.213	−248.065	−6.752	0.077
4700	40.439	339.976	304.390	167.251	−250.158	−1.483	0.016
4800	40.563	340.828	305.141	171.301	−252.335	3.830	−0.042
4900	40.687	341.666	305.878	175.363	−254.603	9.191	−0.098
5000	40.812	342.489	306.602	179.438	−256.971	14.598	−0.153
5100	40.935	343.299	307.313	183.526	−259.084	20.027	−0.205
5200	41.059	344.095	308.013	187.625	−261.572	25.523	−0.256
5300	41.181	344.878	308.701	191.737	−264.162	31.070	−0.306
5400	41.302	345.649	309.378	195.861	−266.861	36.665	−0.355
5500	41.422	346.408	310.045	199.998	−269.674	42.311	−0.402
5600	41.541	347.155	310.701	204.146	−272.608	48.010	−0.448
5700	41.658	347.892	311.347	208.306	−275.665	53.762	−0.493
5800	41.773	348.617	311.983	212.477	−278.855	59.570	−0.536
5900	41.887	349.332	312.610	216.660	−282.182	65.432	−0.579
6000	41.999	350.037	313.228	220.855	−285.652	71.353	−0.621

PREVIOUS: December 1973 (1 atm) CURRENT. December 1973 (1 bar)

Chromium Oxide (CrO) **$Cr_1O_1(g)$**

Chromium Oxide (CrO_2) IDEAL GAS $M_r = 83.9948$ Chromium Oxide (CrO_2) $Cr_1O_2(g)$

$\Delta_fH°(0\ K) = -73.78 \pm 41.8\ kJ \cdot mol^{-1}$

$S°(298.15\ K) = 269.24 \pm 12.6\ J \cdot K^{-1} \cdot mol^{-1}$ $\Delta_fH°(298.15\ K) = -75.31 \pm 41.8\ kJ \cdot mol^{-1}$

Vibrational Frequences and Degeneracies υ, cm^{-1}
998 (1)
[300](1)
1008 (1)

Ground State Quantum Weight: [3] $\sigma = 2$
Point Group : [C_{2v}]
Bond Distance: Cr–O = [1.627] Å
Bond Angle: O–Cr–O = [110]°
Product of the Moments of Inertia: $I_AI_BI_C = [3.326337 \times 10^{-115}]\ g^3 \cdot cm^6$

Enthalpy of Formation

Grimley *et al.*[1] studied the vaporization of $Cr_2O_3(cr)$ under neutral and oxidizing conditions using mass spectrometric methods. In the range 1842–2062 K (IPTS–68) this study detected quantitatively Cr(g), CrO(g), $CrO_2(g)$, O(g), and $O_2(g)$. Of the many chemical equilibria which could be analyzed, we tabulated below our 2nd and 3rd law analyses of the equilibrium between CrO(g) and $CrO_2(g)$.

	$\Delta rH°(298.15\ K)$, $kcal \cdot mol^{-1}$ 2nd law	$\Delta rH°(298.15\ K)$, $kcal \cdot mol^{-1}$ 3rd law	Drift $cal \cdot K^{-1} \cdot mol^{-1}$	$\Delta_fH°(298.15\ K)$, $kcal \cdot mol^{-1}$
Neutral system, 13 points, 1843–2062 K				
Reaction A**	141.27	119.87	−10.9 ± 3.6	−15.31
Reaction B**	71.11	64.41	−3.4 ± 2.8	−19.41
Oxidizing system, 3 points, 1893–1945 K				
Reaction A	120.97	122.48	0.8 ± 9.2	−17.92
Reaction B	101.21		−17.9 ± 0.1	−21.82

** One point (1865 K) rejected due to a statistical test.
Reactions: (A) $CrO_2(g) = CrO(g) + O(g)$. (B) $CrO_2(g) = CrO(g) + 1/2\ O_2(g)$.

We adopt $\Delta_fH°(298.15\ K) = -18.0 \pm 10.0\ kcal \cdot mol^{-1}$ ($-75.312 \pm 41.8\ kJ \cdot mol^{-1}$). This value is intermediate to the four results tabulated above with extra weight given to those of the neutral conditions. Our analysis of equations analogous to those treated in the CrO(g) table[3] yields the same trends as with CrO(g). The results are consistent with our adopted value.

Using auxiliary data,[3] we calculate $\Delta_{a}H° = 9.98$ eV (230.1 $kcal \cdot mol^{-1}$) corresponding to $CrO_2(g) = Cr(g) + 2\ O(g)$. This value is a factor of 2.12 greater than $D_0^\circ(CrO,g)$.[3]

Chizhikov *et al.*[2] also studied the vaporization of Cr_2O_3 via mass spectrometry in the range 1690–2020 K. They reported the detection of gaseous Cr, CrO, CrO_2, and O during the evaporation process. The reported smoothed partial pressures of CrO(g) and $CrO_2(g)$ lie higher than those of Grimley *et al.*[1] by a factor of 2–5, while the partial pressures of Cr(g) are less than a factor of two difference. This study was not further analyzed.

Mass spectrometric studies were made by Farber and Srivastava[7] on the reactions involved with vanadium and chromium additives in potassium–seeded H_2/O_2 flames. Equilibrium values at an average flame temperature of 2250 K for the reaction for $CrO_2(g) + 2\ H_2O(g) = H_2CrO_4(g) + 2\ H(g)$ were analyzed by Farber and Srivastava.[7] They calculated $\Delta_fH°(298.15\ K) = -3.0 \pm 7\ kcal \cdot mol^{-1}$ for $CrO_2(g)$. The experimental determination of $\Delta_fH°(298.15\ K)$ for $H_2CrO_4(g)$ also required the $\Delta_fH°(298.15\ K)$ value for CrO(g). Adjusting the calculations of Farber and Srivastava[7] to be consistent with the JANAF $\Delta_fH°(298.15\ K)$ value for CrO(g),[3] we recalculate $\Delta_fH°(298.15\ K) = -11.0\ kcal \cdot mol^{-1}$ for $CrO_2(g)$.

Heat Capacity and Entropy

$CrO_2(g)$ is assumed to have a molecular geometry similar to that observed for $TiO_2(g)$, $ZrO_2(g)$, and $TaO_2(g)$.[3] The O–Cr–O bond is estimated as 110° while the Cr–O bond distance is estimated to be the same as that in CrO(g) [3]. The symmetric and asymmetric stretching frequencies are obtained from the infrared spectra of gaseous tetrahedral CrO_2Cl_2 and CrO_2F_2.[4, 5] The bending frequency of 300 cm^{-1} is estimated, based on analogies with $TaO_2(g)$ and $WO_2(g)$.[3 6] Refer also to the TiO_2ideal gas table.[3] The electronic ground state is assumed to be $^3A_1$ as in $WO_2(g)$.[6] The principal moments of inertia are: $I_A = 2.8646 \times 10^{-39}$, $I_B = 9.4383 \times 10^{-39}$, and $I_C = 12.3029 \times 10^{-39} g \cdot cm^2$.

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

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	S° (J·K⁻¹mol⁻¹)	−[G°−H°(T_r)]/T (J·K⁻¹mol⁻¹)	H°−H°(T_r) (kJ·mol⁻¹)	$\Delta_fH°$ (kJ·mol⁻¹)	$\Delta_fG°$ (kJ·mol⁻¹)	log K_f
0	0.	0.	INFINITE	−11.210	−73.781	−73.781	INFINITE
100	35.384	226.805	305.163	−7.836	−73.623	−78.544	41.027
200	39.615	252.725	273.086	−4.072	−74.354	−83.229	21.737
250	41.517	261.768	269.945	−2.044	−74.844	−85.391	17.842
298.15	43.390	269.241	269.241	0.	−75.312	−87.380	15.309
300	43.461	269.510	269.242	0.080	−75.329	−87.455	15.227
350	45.324	276.351	269.778	2.301	−75.887	−89.426	13.346
400	47.010	282.515	270.991	4.610	−76.313	−91.331	11.927
450	48.482	288.139	272.588	6.998	−76.723	−93.184	10.816
500	49.742	293.315	274.406	9.454	−77.124	−94.991	9.924
600	51.712	302.568	278.347	14.533	−77.924	−98.490	8.574
700	53.121	310.651	282.396	19.778	−78.748	−101.852	7.600
800	54.142	317.814	286.385	25.144	−79.618	−105.095	6.862
900	54.896	324.237	290.240	30.598	−80.564	−108.223	6.281
1000	55.464	330.052	293.935	36.117	−81.623	−111.241	5.811
1100	55.902	335.360	297.463	41.686	−82.829	−114.145	5.420
1200	56.245	340.239	300.827	47.294	−84.201	−116.933	5.090
1300	56.518	344.752	304.034	52.933	−85.760	−119.599	4.806
1400	56.738	348.949	307.095	58.596	−87.521	−122.137	4.557
1500	56.918	352.870	310.017	64.279	−89.495	−124.543	4.337
1600	57.068	356.548	312.811	69.979	−91.689	−126.809	4.140
1700	57.193	360.012	315.487	75.692	−94.109	−128.931	3.962
1800	57.298	363.284	318.052	81.417	−96.760	−130.904	3.799
1900	57.388	366.384	320.515	87.151	−99.647	−132.723	3.649
2000	57.466	369.330	322.883	92.894	−102.774	−134.384	3.510
2100	57.532	372.135	325.162	98.644	−106.144	−135.883	3.380
2200	57.591	374.813	327.358	104.400	−129.096	−136.559	3.242
2300	57.642	377.374	329.478	110.162	−131.098	−136.854	3.108
2400	57.686	379.828	331.525	115.928	−133.117	−137.062	2.983
2500	57.726	382.184	333.504	121.699	−135.155	−137.184	2.866
2600	57.761	384.449	335.421	127.473	−137.209	−137.225	2.757
2700	57.793	386.629	337.277	133.251	−139.282	−137.186	2.654
2800	57.821	388.732	339.077	139.032	−141.372	−137.070	2.557
2900	57.847	390.761	340.825	144.815	−143 479	−136.880	2.465
3000	57.870	392.723	342.522	150.601	−484.621	−132.003	2.298
3100	57.890	394.620	344.172	156.389	−485.933	−120.227	2.026
3200	57.909	396.459	345.778	162.179	−487.312	−108.409	1.770
3300	57.927	398.241	347.341	167.971	−488.755	−96.546	1.528
3400	57.942	399.970	348.863	173.764	−490.260	−84.638	1.300
3500	57.957	401.650	350.348	179.559	−491.827	−72.686	1.085
3600	57.970	403.283	351.795	185.355	−493.455	−60.687	0.881
3700	57.982	404.872	353.209	191.153	−495.143	−48.643	0.687
3800	57.994	406.418	354.589	196.952	−496.893	−36.552	0.502
3900	58.004	407.925	355.937	202.752	−498.705	−24.414	0.327
4000	58.014	409.393	357.255	208.553	−500.582	−12.229	0.160
4100	58.023	410.826	358.544	214.354	−502.526	0.004	−0.000
4200	58.031	412.224	359.806	220.157	−504.540	12.285	−0.153
4300	58.039	413.590	361.041	225.961	−506.629	24.615	−0.299
4400	58.046	414.924	362.250	231.765	−508.796	36.994	−0.439
4500	58.053	416.229	363.435	237.570	−511.046	49.423	−0.574
4600	58.059	417.505	364.597	243.375	−513.386	61.903	−0.703
4700	58.065	418.753	365.736	249.182	−515.821	74.436	−0.827
4800	58.071	419.976	366.853	254.988	−518.359	87.021	−0.947
4900	58.076	421.173	367.950	260.796	−521.007	99.661	−1.062
5000	58.081	422.347	369.026	266.603	−523.773	112.356	−1.174
5100	58.085	423.497	370.083	272.412	−526.302	125.080	−1.281
5200	58.090	424.625	371.121	278.221	−529.225	137.879	−1.385
5300	58.094	425.731	372.141	284.030	−532.269	150.738	−1.486
5400	58.098	426.817	373.143	289.839	−535.442	163.654	−1.583
5500	58.102	427.883	374.129	295.649	−538.748	176.630	−1.677
5600	58.105	428.930	375.098	301.460	−542.195	189.669	−1.769
5700	58.108	429.959	376.052	307.270	−545.786	202.769	−1.858
5800	58.112	430.969	376.990	313.081	−549.530	215.934	−1.945
5900	58.114	431.963	377.913	318.893	−553.433	229.164	−2.029
6000	58.117	432.940	378.822	324.704	−557.500	242.463	−2.111

PREVIOUS: December 1973 (1 atm) CURRENT· December 1973 (1 bar)

Chromium Oxide (CrO_3) IDEAL GAS $M_r = 99.9942$ Chromium Oxide (CrO_3) $Cr_1O_3(g)$

$S°(298.15\ K) = [266.2 \pm 16.7]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$

$\Delta_f H°(0\ K) = -288.2 \pm 41.8\ kJ{\cdot}mol^{-1}$
$\Delta_f H°(298.15\ K) = -292.88 \pm 41.8\ kJ{\cdot}mol^{-1}$

Vibrational Frequencies and Degeneracies v, cm^{-1}
[875](1)
[500](1)
969 (2)
[425](2)

Ground State Quantum Weight: [1]
Point Group: [D_{3h}]
Bond Distance: Cr–O = [1.627] Å
Bond Angle: O–Cr–O = [120]°
Product of the Moments of Inertia = $I_A I_B I_C = [2.348053 \times 10^{-114}]\ g^3{\cdot}cm^6$

Enthalpy of Formation

The vaporization of Cr_2O_3 under oxidizing conditions was studied by Grimley, Burns, and Inghram[1] using mass spectrometric methods. The principal gaseous species observed were Cr, CrO, CrO_2, CrO_3, O, and O_2. The vapor pressures at three different temperatures (1893, 1914, and 1942 K, IPTS–68) are analyzed for four different reactions by the 2nd and 3rd law methods.

Reaction	$\Delta_r H°(298.15\ K)$, $kcal{\cdot}mol^{-1}$ 2nd law	3rd law	Drift $cal{\cdot}K^{-1}{\cdot}mol^{-1}$	$\Delta_f H°(298.15\ K)$ $kcal{\cdot}mol^{-1}$
$Cr(g) + 3\ O(g) = CrO_3(g)$	−279.80	−332.47	−27.5 ± 6.4	−58.79
$Cr(g) + 1.5\ O_2(g) = CrO_3(g)$	−220.52	−165.48	28.7 ± 21.1	−70.48
$0.5\ Cr_2O_3(cr) + 1.5\ O(g) = CrO_3(g)$	−30.81	−24.28	3.4 ± 1.4	−70.04
$0.5\ Cr_2O_3(cr) + 0.75\ O_2(g) = CrO_3(g)$	−1.17	59.22	31.5 ± 12.4	−75.88

The 2nd law results are considered less reliable due to the small number of data points and the small temperature range studied (52 K). We adopt $\Delta_f H°(CrO_3, g, 298.15\ K) = -70.0 \pm 10\ kcal\ mol^{-1}$ ($-292.880 \pm 41.8\ kJ{\cdot}mol^{-1}$).

Washburn,[3] in a mass spectrometric study of the sublimation of $CrO_3(cr)$, stated that the gaseous Cr–containing molecules are in equilibrium among themselves but not with O(g). If the same situation were to hold in the study by Grimley *et al.*,[1] a value intermediate to −70.04 and $-75.88\ kcal{\cdot}mol^{-1}$ might be more appropriate. However, the adopted value with its assigned uncertainty is still consistent with this possibility.

Mass spectrometric studies were made by Farber and Srivastava[6] on the reactions involved with vanadium and chromium additives in potassium–seeded H_2/O_2 flames. Equilibrium values at an average flame temperature of 2250 K for the reaction $CrO_3(g) + H_2O(g) = H_2CrO_4(g)$ were analyzed by Farber and Srivastava.[6] They calculated $\Delta_f H°(298.15\ K) = -64.6 \pm 7\ kcal{\cdot}mol^{-1}$ for $CrO_3(g)$. The experimental determination of $\Delta_f H°(298.15\ K)$ for $H_2CrO_4(g)$ also required the $\Delta_f H°(298.15\ K)$ value for CrO(g). Adjusting the calculations of Farber and Srivastava[6] to be consistent with the JANAF $\Delta_f H°(298\ 15\ K)$ value for CrO(g),[2] we recalculate $\Delta_f H°(289.15\ K) = -72.6\ kcal{\cdot}mol^{-1}$ for $CrO_3(g)$.

Defining the dissociation by $CrO_3(g) = Cr(g) + 3O(g)$, we calculate $\Delta_{at}H° = 14.8 \pm 0.4\ eV$ ($340.3 \pm 10\ kcal{\cdot}mol^{-1}$). This compares with $D_0^\circ = 4.71\ eV$ for CrO(g) and $\Delta_{at}H° = 9.98\ eV$ for $CrO_2(g)$ for similar dissociations.[2]

Heat Capacity and Entropy

The molecular structure is assumed to be planar with D_{3h} symmetry. The three Cr–O bond distances are taken to be the same as in CrO(g).[2] The principal moments of inertia are $I_A = I_B = 10.5494 \times 10^{-39}$ and $I_C = 21.0987 \times 10^{-39}\ g{\cdot}cm^2$.

Barraclough *et al.*[4] observed a vibrational frequency at 969 cm^{-1} in the infrared spectrum of $CrO_3(cr)$ dispersed in a Nujol mull. This frequency was assigned to represent the stretching frequency of the two free Cr–O groups in crystalline CrO_3. We assume this frequency also represents the stretching mode in the vapor phase. This infrared work is supported by the infrared and Raman studies of Mattes.[5] The remaining vibrational frequencies are those suggested by Grimley *et al.*[1] The electronic ground state is assumed to be a singlet.

References

[1] R. F. Grimley, R. P. Burns, and M. G. Inghram, J. Chem. Phys. 34, 664 (1961).
[2] JANAF Thermochemical Tables: CrO(g) and $CrO_2(g)$, 12–31–73.
[3] C. A. Washburn, U. S. Clearinghouse Fed. Sci. Tech. Inform., PB–183562 (1969); Chem. Abstr. 71, 755276 (1969).
[4] C. G. Barraclough, J. Lewis and R. S. Nyholm, J. Chem. Soc. 1959, 3552 (1959).
[5] R. Mattes, Z. Naturforsch B24, 772 (1969).
[6] M. Farber and R. D. Srivastava, Combustion and Flame 20, 43 (1973).

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

	$J{\cdot}K^{-1}mol^{-1}$			$kJ{\cdot}mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−12.379	−288.176	−288.176	INFINITE
100	34.969	218.552	308.811	−9.026	−289.492	−284.922	148.828
200	45.791	245.909	270.989	−5.016	−291.432	−279.595	73.023
250	51.301	256.729	267.075	−2.586	−292.250	−276.538	57.779
298.15	56.025	266.178	266.178	0.	−292.880	−273.452	47.908
300	56.193	266.525	266.179	0 104	−292.901	−273.332	47.591
350	60.366	275.510	266.879	3.021	−293.500	−270.016	40.298
400	63.839	283.805	268.483	6.129	−293.875	−266.634	34.819
450	66.695	291.495	270.618	9.394	−294.165	−263.211	30.553
500	69.037	298.647	273.068	12.790	−294.399	−259.759	27.137
600	72.542	311.564	278.431	19.880	−294.767	−252.795	22.008
700	74.953	322.939	283.993	27.262	−295.082	−245.774	18.340
800	76.658	333.065	289.506	34.847	−295.401	−238.709	15.586
900	77.896	342.169	294.860	42.578	−295.772	−231.601	13.442
1000	78.819	350.426	300.010	50.416	−296.243	−224.447	11.724
1100	79.523	357.973	304.942	58.335	−296.854	−217.239	10.316
1200	80.071	364.917	309.654	66.315	−297.628	−209.968	9.140
1300	80.505	371.344	314.155	74.345	−298.587	−202.626	8.142
1400	80.855	377.323	318.456	82.414	−299.750	−195.202	7.283
1500	81.140	382.912	322.569	90.514	−301.128	−187.688	6.536
1600	81.375	388.156	326.506	98.640	−302.729	−180.074	5.879
1700	81.572	393.095	330.279	106.787	−304.560	−172.353	5.296
1800	81 738	397 763	333 900	114.953	−306.628	−164.518	4 774
1900	81.879	402.186	337.379	123.134	−308.939	−156.561	4.304
2000	82.000	406.389	340.725	131.328	−311.496	−148.476	3.878
2100	82.104	410.392	343.948	139.534	−314.303	−140.257	3.489
2200	82.195	414.214	347.055	147.749	−336.700	−131.242	3.116
2300	82.275	417.869	350.055	155.972	−338.155	−121.871	2.768
2400	82.345	421.373	352.955	164.203	−339.637	−112.437	2.447
2500	82.406	424.735	355.759	172.441	−341.144	−102.939	2.151
2600	82.461	427.968	358.474	180.684	−342.678	−93.381	1.876
2700	82.511	431.081	361.106	188.933	−344.238	−83.762	1.620
2800	82.555	434.083	363.659	197.186	−345.825	−74.086	1.382
2900	82.594	436.981	366.138	205.444	−347.436	−64.353	1.159
3000	82.630	439.781	368.546	213.705	−688.092	−49.951	0.870
3100	82.662	442.491	370.888	221.970	−688.925	−28.665	0.483
3200	82.692	445.116	373.167	230.237	−689.833	−7.353	0.120
3300	82.718	447.661	375.386	238.508	−690.813	13.989	−0.221
3400	82.743	450.131	377.548	246.781	−691.862	35.363	−0.543
3500	82.765	452.530	379.657	255.056	−692.981	56.767	−0.847
3600	82 786	454.862	381.713	263.334	−694.166	78.206	−1.135
3700	82.805	457.130	383.721	271.613	−695.420	99.677	−1.407
3800	82.823	459.339	385.682	279.895	−696.741	121.185	−1.666
3900	82.839	461.490	387.598	288.178	−698.131	142.728	−1.912
4000	82.854	463.588	389.472	296.463	−699.592	164.306	−2.146
4100	82.868	465.634	391.305	304.749	−701.126	185.922	−2.369
4200	82.881	467.631	393.098	313.036	−702.736	207.577	−2.582
4300	82.893	469.581	394.854	321.325	−704.427	229.271	−2.785
4400	82.904	471.487	396.575	329.615	−706.201	251.005	−2.980
4500	82.914	473.350	398.260	337.906	−708.065	272.780	−3.166
4600	82.924	475.173	399.912	346.197	−710.023	294.597	−3.345
4700	82.934	476.956	401.533	354 490	−712.083	316.459	−3.517
4800	82.942	478.702	403.122	362.784	−714.251	338.366	−3.682
4900	82.950	480.413	404.682	371.079	−716.536	360.320	−3.841
5000	82.958	482.088	406.214	379.374	−718.944	382.321	−3.994
5100	82.965	483.731	407.718	387.670	−721.123	404.344	−4.141
5200	82.972	485.342	409.195	395.967	−723.702	426.436	−4.284
5300	82.978	486.923	410.647	404.265	−726.409	448.581	−4.421
5400	82.984	488.474	412.074	412.563	−729.253	470.776	−4.554
5500	82.990	489.997	413.476	420.862	−732.237	493.025	−4.682
5600	82.996	491.492	414.856	429.161	−735.371	515.332	−4.807
5700	83.001	492.961	416.214	437.461	−738.658	537.694	−4.927
5800	83.006	494.405	417.549	445.761	−742.106	560.117	−5.044
5900	83.010	495.824	418.864	454.062	−745.723	582.598	−5.158
6000	83.015	497.219	420.158	462.363	−749.514	605.145	−5.268

PREVIOUS: December 1973 (1 atm) — CURRENT December 1973 (1 bar)

Chromium Oxide (CrO_3) $Cr_1O_3(g)$

Chromium Nitride (Cr$_2$N) CRYSTAL $M_r = 117.9987$ Chromium Nitride (Cr$_2$N) Cr$_2$N$_1$(cr)

$\Delta_f H°(0\ \mathrm{K})$ = Unknown

$S°(298.15\ \mathrm{K}) = [64.85 \pm 8.4]\ \mathrm{J{\cdot}K^{-1}{\cdot}mol^{-1}}$ $\Delta_f H°(298.15\ \mathrm{K}) = -125.52 \pm 12.6\ \mathrm{kJ{\cdot}mol^{-1}}$

Enthalpy of Formation

Mah[1] has measured the enthalpy of combustion of chromium subnitride at 303.15 K. From her data for the process $Cr_2N_{0.969}(cr) + 1.5O_2(g) = Cr_2O_3(cr) + 0.4845\ N_2(g)$, we calculate $\Delta_c H°(298.15\ \mathrm{K}) = -241.29 \pm 1.5\ \mathrm{kcal{\cdot}mol^{-1}}$ at unit fugacities of oxygen and nitrogen. Impurity corrections are based on JANAF enthalpy of formation data.[2] When the value for $\Delta_c H°$ is combined with the enthalpy of formation for Cr_2O_3,[2] one obtains $\Delta_f H°(Cr_2N_{0.969}, cr, 298.15\ \mathrm{K}) = -29.9 \pm 3.5\ \mathrm{kcal{\cdot}mol^{-1}}$. The large uncertainty arises from impurities in the subnitride sample, as well as from the uncertainty ($\pm 2.0\ \mathrm{kcal{\cdot}mol^{-1}}$) in the $\Delta_f H°$ of Cr_2O_3.[2]

All available equilibrium nitrogen pressures except those of one study[5] have been recently for the reaction $2\ Cr(cr) + 0.5\ N_2(g) = Cr_2N(cr)$. These results are reanalyzed by the 2nd and 3rd law methods using revised thermal functions for Cr_2N (see below). We have not taken into account in our analysis any variations in the composition of the subnitride.

Source	Data Points	T/K	Drift $\mathrm{cal{\cdot}K^{-1}{\cdot}mol^{-1}}$	$\Delta_f H°(298.15\ \mathrm{K})$, $\mathrm{kcal{\cdot}mol^{-1}}$ 2nd law	3rd law
Sano[4]	6	1229–1395	−3.7 ± 0.2	−24.0	−28.8 ± 0.5
Mozgovai and Samarin[5]	Equation	1600–1750	−14.0	−10.2	−33.8 ± 1.7
Seybolt and Oriani[6]	5	1273–1673	−7.8 ± 5.4	−21.3	−32.8 ± 3.9
Tomilin and Savost'yanova[7]	Equation	1517–1724	−32.6	−20.3	−32.6 ± 5.7
Mills[8]	Equation	1337–1653	−2.1	−29.2	−32.3 ± 0.5
Schwerdtfeger[9]	3	1373–1583	−3.7 ± 0.7	−27.1	−32.5 ± 0.8
Smith[10]	2	1333–1370	−13.4	−13.6	−31.7 ± 0.7

We adopt $\Delta_f H°(Cr_2N, cr, 298.15\ \mathrm{K}) = -30.0 \pm 3.0\ \mathrm{kcal{\cdot}mol^{-1}}$ ($-125.52 \pm 12.6\ \mathrm{kJ{\cdot}mol^{-1}}$) which is based on the 2nd and 3rd law results from the two equilibrium studies[8,9] and the $\Delta_f H°$ value determined by combustion calorimetry.[1] Our adopted value agrees with that selected by NBS (−30.5)[11] but is 1.8 kcal·mol⁻¹ less negative than the selected value of DeLuca and Leitnaker.[3]

Heat Capacity and Entropy

No low temperature heat capacity data for Cr_2N have been reported. By analogy with entropies[2,12,13] for other transition–metal subnitrides, for the reaction $2\ M(cr) + 0.5\ N_2(g) = M_2N(cr)$ where M=Fe, Mo, Nb, Ta, and V, we calculate an average $\Delta_r S°$ of $-18.7\ \mathrm{cal{\cdot}K^{-1}{\cdot}mol^{-1}}$. This value is combined with entropies for Cr and N_2[2] to give $15.5\ \mathrm{cal{\cdot}K^{-1}{\cdot}mol^{-1}}$ as $S°(298.15\ \mathrm{K})$ for $Cr_2N(cr)$. Other reported estimates in $\mathrm{cal{\cdot}K^{-1}{\cdot}mol^{-1}}$ for $S°(298.15\ \mathrm{K})$ are 14.3[3] and 17.7 ± 1.0.[14]

The only high temperature enthalpy study reported for Cr_2N is that of Satoh,[15] who measured heat contents $[H°(T)-H°(273.15\ \mathrm{K})]$ three nitride samples at three temperatures each (372.6, 598.8, and 784.2 K) in an ice calorimeter. DeLuca and Leitnaker[3] have shown that the subnitride sample used by Satoh[15] was substoichiometric, reevaluated his heat contents and presented $C_p°$ data for Cr_2N in the temperature range 298–1800 K. A comparison of their value ($17.0\ \mathrm{cal{\cdot}K^{-1}{\cdot}mol^{-1}}$) for $C_p°(298.15\ \mathrm{K})$ with similar data for other transition–metal subnitrides[2,12,13] indicates it is probably too large by $1\text{–}2\ \mathrm{cal{\cdot}K^{-1}{\cdot}mol^{-1}}$. We find a $\Delta_f C_p$ of $1.1\ \mathrm{cal{\cdot}K^{-1}{\cdot}mol^{-1}}$ for several subnitrides[2,12,13] which leads to a $C_p°$ value of $15.79\ \mathrm{cal{\cdot}K^{-1}{\cdot}mol^{-1}}$ for Cr_2N at 298.15 K. This value is adopted and joined smoothly with the data of Deluca and Leitnaker[3] near 400 K. $C_p°$ data above 1800 K are obtained by graphical extrapolation.

Phase Data

Blix[16] has determined the structure of the subnitride phase as hexagonal by x–ray diffraction methods, and he indicated that the homogeneity limits extend from $CrN_{0.47}$ to $CrN_{0.66}$. Eriksson[17] has reported that the phase exists between $CrN_{0.38}$ and $CrN_{0.50}$. Mills,[8] using a thermogravimetric technique, has examined the homogeneity limits of Cr_2N as a function of temperature. The upper limiting composition was determined to be $CrN_{0.49}$ with only a small variation with temperature. The lower limiting composition of Cr_2N varied widely with temperature in the range 1273–1373 K. Mills[8] reported the limiting composition as $CrN_{0.41}$, at 1273 K and $CrN_{0.37}$ at 1373 K. Other information on the chromium–chromium nitride system has been reviewed by Storms.[18]

Decomposition Data

No information is available on the melting point of Cr_2N. We assume that the subnitride decomposes prior to melting, according to the reaction $Cr_2N(cr) \rightarrow 2\ Cr(cr) + 0.5\ N_2(g)$. T_{dcm} is the temperature at which $\Delta_r G°$ for the decomposition process equals zero.

References

[1] A. D. Mah, U. S. Bur. Mines RI 5529, (1960).
[2] JANAF Thermochemical Tables: $N_2(g)$, 9–30–66, Cr(cr), 6–30–73; $Cr_2O_3(cr)$ and $VN_{0.465}(cr)$, 12–31–73.
[3] J. P. DeLuca and J. M. Leitnaker, J. Amer. Ceram. Soc. 56, 126 (1973).
[4] K. Sano, Nippon Kagaku Kaishi 58, 981 (1937).

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

T/K	$C_p°$ (J·K⁻¹mol⁻¹)	$S°$ (J·K⁻¹mol⁻¹)	$-[G°-H°(T_r)]/T$ (J·K⁻¹mol⁻¹)	$H°-H°(T_r)$ (kJ·mol⁻¹)	$\Delta_f H°$ (kJ·mol⁻¹)	$\Delta_f G°$ (kJ·mol⁻¹)	log K_f
0							
100							
200							
298.15	66.065	64.852	64.852	0.	−125.520	−102.208	17.906
300	66.191	65.261	64.853	0.122	−125.511	−102.063	17.771
400	73.429	85.388	67.548	7.136	−125.040	−94.280	12.312
500	76.735	102.139	72.841	14.649	−124.190	−86.688	9.056
600	79.496	116.373	78.939	22.460	−123.309	−79.270	6.901
700	82.257	128.835	85.195	30.548	−122.371	−72.003	5.373
800	84.977	139.996	91.359	38.910	−121.362	−64.876	4.236
900	87.738	150.165	97.336	47.546	−120.304	−57.878	3.359
1000	90.500	159.552	103.094	56.457	−119.244	−50.999	2.664
1100	93.261	168.307	108.629	65.646	−118.236	−44.224	2.100
1200	95.981	176.538	113.949	75.108	−117.311	−37.537	1.634
1300	98.742	184.330	119.066	84.844	−116.500	−30.923	1.243
1400	101.504	191.749	123.994	94.856	−115.828	−24.366	0.909
1500	104.265	198.846	128.749	105.145	−115.305	−17.853	0.622
1600	107.027	205.663	133.345	115.709	−114.942	−11.369	0.371
1700	109.788	212.235	137.793	126.550	−114.746	−4.902	0.151
1800	112.508	218.589	142.106	137.669	−114.722	1.558	−0.045
1900	114.767	224.731	146.294	149.029	−114.912	8.022	−0.221
2000	117.487	230.688	150.366	160.644	−115.306	14.501	−0.379
2100	119.955	236.479	154.329	172.514	−115.907	21.006	−0.522
2200	122.591	242.121	158.192	184.644	−155.386	28.854	−0.685
2300	124.934	247.622	161.961	197.020	−152.693	37.169	−0.844
2400	127.277	252.989	165.643	209.630	−149.771	45.362	−0.987
2500	129.704	258.233	169.242	222.479	−146.617	53.428	−1.116

PREVIOUS: CURRENT: December 1973

Chromium Oxide (Cr_2O_3) CRYSTAL M_r = 151.9902

$S°(298.15\ K) = 81.15 \pm 1.3\ J{\cdot}K^{-1}{\cdot}mol^{-1}$
$T_{fus} = 2603 \pm 15\ K$

$\Delta_fH°(0\ K) = -1128.84 \pm 8.4\ kJ{\cdot}mol^{-1}$
$\Delta_fH°(298.15\ K) = -1134.70 \pm 8.4\ kJ{\cdot}mol^{-1}$
$\Delta_{fus}H° = [129.7]\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

Two oxygen bomb calorimetric studies on Cr(cr) led to reported values of $\Delta_fH°(Cr_2O_3$, cr, 298.15 K) = −272.6 ± 0.4 kcal·mol^{-1} by Mah[1] and −271.0 ± 1.8 kcal·mol^{-1} by Golutvin and Chin'k'uei.[2] Mah[1] reported that completions of combustion ranged from 95.30 to 98.90% and applied corrections. Of the fourteen runs by Golutvin and Chin'k'uei,[2] seven had a completeness of combustion of 91.88 to 98.96%. Their reported $\Delta_fH°$(298.15 K) value is based on an average of the results for these seven runs with no correction for incomplete combustion or impurities. These latter authors[2] also stated that there was no clear dependence between the enthalpy of combustion and completeness of combustion. Early calorimetric studies led to reported values for $\Delta_fH°$ of −267.8 (298 K),[3] −288.9 ± 1.0 (292 K),[4] and −268.9 ± 0.6 kcal·mol^{-1} (294 K).[5]

There are many equilibrium studies involving Cr_2O_3(cr). Our analysis of the more recent studies are tabulated below. The free energy of formation equation presented by Richardson and Jeffes[8] is representative of the earlier equilibrium studies.[9]

Source	Reaction	T/K	Data Points	$\Delta_fH°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law	Drift cal·K^{-1}·mol^{-1}	$\Delta_fH°$(298.15 K), kcal·mol^{-1} 2nd law	3rd law
8	A	873–1773	Eqn.	−270.62	−268.44	1.7	−270.62	−268.44
9	B(transpiration)	871–1427	4	−32.89 ± 0.65	−31.61 ± 0.65	1.1 ± 0.5	−272.05	−268.22
10	B(static)	1313–1573	5(47)	−32.17 ± 0.75	−32.36 ± 0.19	−0.1 ± 0.5	−269.89	−270.46
11	B(transpiration)	1493–1893	5	−32.85 ± 0.94	−32.79 ± 0.30	0.1 ± 0.6	−271.94	−271.76
12	A(emf)	1000–1700	Eqn.	−264.60	−268.91	−3.3	−264.60	−268.91
13	A(emf)	1173–1523	Eqn.	−269.71	−270.32	−0.5	−269.71	−270.32

Reactions. (A) 2 Cr(cr) + 3/2 O_2(g) = Cr_2O_3(cr). (B) 2/3 Cr(cr) + H_2O(g) = 1/3 Cr_2O_3(cr) + H_2(g).

We adopt $\Delta_fH°(Cr_2O_3$, cr, 298.15 K) = −271.2 ± 2.0 kcal·mol^{-1} (1134.701 ± 8.4 kJ·mol^{-1}). This value is an average of two combustion studies,[1,2] and three equilibrium studies which have a small third law drift.[10, 11, 13]

Kelly *et al.*[6] investigated experimentally the thermodynamic properties of the chromium carbides. They measured the CO(g) equilibrium pressure in four distinct systems. A combination of our analyses of these four equilibria[7] leads to $\Delta_fH°(Cr_2O_3$, cr, 298.15 K) = −269.9 kcal·mol^{-1}.

Heat Capacity and Entropy

The heat capacity of Cr_2O_3(cr) was measured by Anderson [14 (56–336 K)] and by Volger (graph, 100–350 K).[15] Using the combination of Debye and Einstein functions suggested by Anderson,[14] we calculate $S°$(50 K) = 0.386 cal·K^{-1}mol^{-1} and $H°$(50 K) = 14.3 cal·mol^{-1}. Both studies[14, 15] indicated a maximum in the $C_p°$ curve at 205 K. The data of Volger[15] lies considerably higher than that of Anderson.[14] Early heat capacity data by Russell (137–299 K)[16] is in good agreement with that of Anderson.[14] Above 305 K the heat capacity values decrease rapidly (~cal·K^{-1}·mol^{-1}) until 325–340 K, at which point the values show little change with temperature. The adopted $C_p°$ values below T = 330 K are based on the study by Anderson.[14]

Enthalpy data on Cr_2O_3(cr) were measured by Kelley *et al.* (298–1774 K)[6] and Laschschenko and Kompanskii (288–1428 K).[17] The adopted heat capacity values are those suggested by Kelley *et al.*,[6] except that the values in the region 350–500 K are shifted slightly so as to join smoothly with the low temperature heat capacity results.[14] The derived enthalpy values agree with the enthalpy data of Kelley *et al.*[6] to within ±0.5%, the maximum deviation of 25 cal or .5% occurring at 479 K.

Phase Data

Brewer[18] summarized the phase data and reported that Cr_2O_3 has a homogeneity range of x = 1.50–1.56 for CrO_x. Cr_2O_3 has the α–corundum structure and is antiferromagnetic with structural distortion occurring below the Curie temperature of 305 K.

Fusion Data

Refer to the liquid table for details.

References

[1] A. D. Mah, J. Amer. Chem. Soc. 76, 3363 (1954).
[2] Yu. M. Golutvin and L. Chin'k'uei, Russ. J. Phys. Chem. 35, 62 (1961).
[3] W. G. Mixter, Amer. J. Sci. 39, 295 (1915).
[4] W. A. Roth and G. Becker, Z. Physik. Chem. A145, 461 (1929).
[5] W. A. Roth and U. Wolf, Z. Elektrochem. 46, 45 (1940).
[6] K. K. Kelley, F. S. Boericke, G. E. Moore, E. H. Huffman, and W. M. Bangert, U. S. Bur. Mines Tech. Paper 662 (1944).
[7] JANAF Thermochemical Tables: Cr_3C_2(cr), Cr_7C_3(cr), and $Cr_{23}C_6$(cr), 12–31–73.

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Chromium Oxide (Cr_2O_3) Cr_2O_3(cr)

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

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_fH°$ (kJ·mol^{-1})	$\Delta_fG°$ (kJ·mol^{-1})	log K_f
0	0.	0.	INFINITE	−15.282	−1128.844	−1128.844	INFINITE
100	24.255	10.093	155.642	−14.555	−1133.096	−1107.252	578.369
200	75.412	43.065	90.567	−9.501	−1135.576	−1080.195	282.118
298.15	120.366	81.154	81.154	0.	−1134.701	−1053.066	184.493
300	121.922	81.904	81.157	0.224	−1134.645	−1052.560	183.267
305.000	126.775	83.958	81.186	0.845	——— C_p LAMBDA MAXIMUM TRANSITION ———		
305.000	126.775	83.958	81.186	0.845			
400	112.675	113.736	85.534	11.281	−1133.129	−1025.421	133.906
500	117.721	139.503	93.829	22.837	−1131.353	−998.699	104.333
600	120.549	161.232	103.300	34.759	−1129.610	−972.333	84.649
700	122.625	179.977	112.945	46.922	−1127.958	−946.252	70.610
800	124.290	196.463	122.375	59.270	−1126.413	−920.401	60.096
900	125.725	211.187	131.440	71.773	−1125.007	−894.736	51.929
1000	127.009	224.501	140.091	84.410	−1123.795	−869.217	45.403
1100	128.202	236.663	148.325	97.171	−1122.829	−843.808	40.069
1200	129.332	247.867	156.159	110.049	−1122.137	−818.475	35.627
1300	130.411	258.261	163.618	123.036	−1121.754	−793.188	31.871
1400	131.457	267.964	170.729	136.130	−1121.703	−767.918	28.651
1500	132.482	277.069	177.518	149.327	−1121.999	−742.639	25.861
1600	133.486	285.651	184.011	162.625	−1122.654	−717.329	23.418
1700	134.478	293.774	190.230	176.024	−1123.676	−691.967	21.262
1800	135.457	301.486	196.199	189.517	−1125.077	−666.534	19.342
1900	136.880	308.848	201.935	203.135	−1126.833	−641.013	17.623
2000	138.168	315.903	207.459	216.888	−1128.937	−615.391	16.072
2100	139.056	322.665	212.785	230.749	−1131.423	−589.654	14.667
2200	139.947	329.155	217.928	244.699	−1172.985	−562.478	13.355
2300	140.839	335.395	222.900	258.739	−1172.557	−534.738	12.144
2400	141.733	341.408	227.714	272.867	−1172.074	−507.017	11.035
2500	142.628	347.212	232.378	287.085	−1171.534	−479.318	10.015
2600	143.526	352.824	236.903	301.393	−1170.937	−451.640	9.074
2603.000	143.553	352.989	237.037	301.824	--- CRYSTAL <--> LIQUID ---		
2700	144.428	358.257	241.298	315.791	−1170.281	−423.987	8.203
2800	145.333	363.526	245.570	330.279	−1169.566	−396.359	7.394
2900	146.242	368.642	249.726	344.857	−1168.789	−368.759	6.642
3000	147.155	373.615	253.773	359.527	−1845.987	−331.960	5.780

PREVIOUS: CURRENT: December 1973

Chromium Oxide (Cr_2O_3) Cr_2O_3(cr)

Chromium Oxide (Cr_2O_3) LIQUID M_r = 151.9902 Chromium Oxide (Cr_2O_3) $Cr_2O_3(l)$

$S°(298.15\ K) = [125.595]\ J{\cdot}K^{-1}{\cdot}mol^{-1}$ $\Delta_fH°(298.15\ K) = [-1018.381]\ kJ{\cdot}mol^{-1}$

$T_{fus} = 2603 \pm 15\ K$ $\Delta_{fus}H° = [129.7]\ kJ{\cdot}mol^{-1}$

Enthalpy of Formation

$\Delta_fH°(Cr_2O_3, l, 298.15\ K)$ is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(2603\ K)-H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The heat capacity for $Cr_2O_3(l)$ is estimated to be $7.5\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$. A glass transition is assumed at 1800 K. Below 1800 K, the $C_p°$ values are those of the crystal with the exception that the values below 500 K are a smooth extrapolation to $C_p° = 24.32\ cal{\cdot}K^{-1}{\cdot}mol^{-1}$ at 298.15 K.

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

Fusion Data

The melting point is chosen to be $T_{fus} = 2603 \pm 15$ K, as suggested by Charlesworth.[1] This result is based on the work by McNally *et al.*[2] The heat of melting is estimated by analogy with $\Delta_{fus}S° = 12.03$ for corundum.[3]

References

[1] J. H. Charlesworth, AFML–TR–70–137, (October 1970).

[2] R. N. McNally, F. I. Peters, and P. H. Ribbs, J. Amer. Ceramic Soc. 44, 491 (1961).

[3] JANAF Thermochemical Tables: $Al_2O_3(cr)$, 6–30–72.

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

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	log K_f
0							
100							
200							
298.15	101.755	125.595	125.595	0.	−1018.381	−949.997	166.435
300	102.006	126.225	125.597	0.188	−1018.361	−949.572	165.335
400	112.717	157.188	129.745	10.977	−1017.113	−926.786	121.026
500	117.721	182.956	137.888	22.534	−1015.337	−904.409	94.483
600	120.549	204.685	147.258	34.456	−1013.593	−882.388	76.819
700	122.625	223.430	156.831	46.619	−1011.942	−860.653	64.223
800	124.290	239.916	166.207	58.967	−1010.396	−839.147	54.791
900	125.725	254.640	175.229	71.469	−1008.991	−817.827	47.465
1000	127.009	267.954	183.847	84.107	−1007.778	−796.654	41.613
1100	128.202	280.116	192.054	96.868	−1006.812	−775.590	36.830
1200	129.332	291.319	199.865	109.745	−1006.121	−754.602	32.847
1300	130.411	301.714	207.305	122.733	−1005.737	−733.660	29.479
1400	131.457	311.417	214.398	135.826	−1005.687	−712.735	26.592
1500	132.482	320.522	221.173	149.024	−1005.983	−691.802	24.091
1600	133.486	329.104	227.653	162.322	−1006.637	−670.838	21.901
1700	134.478	337.227	233.862	175.720	−1007.659	−649.821	19.967
1800	135.457	344.941	239.820	189.217	−1009.056	−628.733	18.245
1800.000	135.457	344.941	239.820	189.217	GLASS <––> LIQUID TRANSITION		
1800.000	156.900	344.941	239.820	189.217			
1900	156.900	353.424	245.578	204.907	−1008.740	−607.615	16.705
2000	156.900	361.472	251.173	220.597	−1008.908	−586.501	15.318
2100	156.900	369.127	256.609	236.287	−1009.566	−565.366	14.063
2200	156.900	376.426	261.891	251.977	−1049.387	−542.878	12.890
2300	156.900	383.401	267.024	267.667	−1047.309	−519.902	11.807
2400	156.900	390.078	272.013	283.357	−1045.265	−497.016	10.817
2500	156.900	396.483	276.864	299.047	−1043.253	−474.213	9.908
2600	156.900	402.637	281.584	314.737	−1041.273	−451.491	9.071
2603.000	156.900	402.818	281.724	315.208	––– CRYSTAL <––> LIQUID –––		
2700	156.900	408.558	286.178	330.427	−1039.325	−428.844	8.296
2800	156.900	414.265	290.651	346.117	−1037.407	−406.268	7.579
2900	156.900	419.770	295.009	361.807	−1035.520	−383.762	6.912
3000	156.900	425.090	299.257	377.497	−1711.697	−352.093	6.130
3100	156.900	430.234	303.400	393.187	−1708.210	−306.830	5.170
3200	156.900	435.216	307.441	408.877	−1704.851	−261.679	4.271
3300	156.900	440.044	311.387	424.567	−1701.615	−216.631	3.429
3400	156.900	444.728	315.240	440.257	−1698.498	−171.678	2.638
3500	156.900	449.276	319.005	455.947	−1695.500	−126.816	1.893
3600	156.900	453.696	322.685	471.637	−1692.618	−82.037	1.190
3700	156.900	457.995	326.285	487.327	−1689.852	−37.338	0.527
3800	156.900	462.179	329.806	503.017	−1687.205	7.291	−0.100
3900	156.900	466.254	333.253	518.707	−1684.678	51.850	−0.694
4000	156.900	470.227	336.628	534.397	−1682.276	96.345	−1.258
4100	156.900	474.101	339.933	550.087	−1680.003	140.782	−1.794
4200	156.900	477.882	343.173	565.777	−1677.867	185.165	−2.303
4300	156.900	481.574	346.349	581.467	−1675.874	229.500	−2.788
4400	156.900	485.181	349.463	597.157	−1674.034	273.788	−3.250
4500	156.900	488.707	352.519	612.847	−1672.356	318.037	−3.692

PREVIOUS· CURRENT: December 1973

Chromium Oxide (Cr_2O_3)

CRYSTAL-LIQUID

0 to 2603 K crystal
above 2603 K liquid

Refer to the individual tables for details.

$M_r = 151.9902$ Chromium Oxide (Cr_2O_3) $Cr_2O_3(cr,l)$

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

T/K	C_p°	S°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−15.282	−1128.844	−1128 844	INFINITE
100	24.255	10.093	155.642	−14.555	−1133.096	−1107.252	578.369
200	75.412	43.065	90.567	−9.501	−1135.576	−1080.195	282.118
298.15	120.366	81 154	81.154	0	−1134.701	−1053.066	184.493
300	121.922	81.904	81.157	0.224	−1134.645	−1052.560	183.267
305 000	126 775	83 958	81.186	0.845	C_p LAMBDA MAXIMUM TRANSITION		
305 000	126.775	83.958	81.186	0.845			
400	112.675	113.736	85.534	11.281	−1133.129	−1025.421	133.906
500	117 721	139.503	93.829	22.837	−1131.353	−998.699	104.333
600	120.549	161.232	103.300	34.759	−1129.610	−972.333	84.649
700	122.625	179.977	112.945	46.922	−1127.958	−946.252	70.610
800	124.290	196.463	122.375	59.270	−1126.413	−920.401	60.096
900	125.725	211.187	131.440	71.773	−1125.007	−894.736	51.929
1000	127.009	224.501	140.091	84.410	−1123.795	−869.217	45.403
1100	128.202	236.663	148.325	97.171	−1122.829	−843.808	40.069
1200	129.332	247.867	156.159	110.049	−1122.137	−818.475	35.627
1300	130.411	258.261	163.618	123.036	−1121.754	−793.188	31.871
1400	131.457	267.964	170.729	136.130	−1121.703	−767.918	28.651
1500	132.482	277.069	177.518	149.327	−1121.999	−742.639	25.861
1600	133.486	285.651	184.011	162.625	−1122.654	−717.329	23 418
1700	134.478	293 774	190.230	176.024	−1123.676	−691.967	21.262
1800	135.457	301.486	196.199	189.517	−1125.077	−666.534	19.342
1900	136.880	308.848	201.935	203.135	−1126.833	−641.013	17.623
2000	138.168	315.903	207.459	216.888	−1128.937	−615.391	16.072
2100	139.056	322.665	212.785	230.749	−1131.423	−589.654	14 667
2200	139.947	329.155	217.928	244.699	−1172.985	−562.478	13.355
2300	140.839	335.395	222.900	258.739	−1172.557	−534.738	12.144
2400	141.733	341.408	227.714	272.867	−1172.074	−507.017	11.035
2500	142.628	347.212	232.378	287.085	−1171.534	−479.318	10.015
2600	143.526	352.824	236.903	301.393	−1170.937	−451 640	9.074
2603.000	143.553	352.989	237.037	301.824	CRYSTAL <--> LIQUID TRANSITION		
2603.000	156.900	402.818	237.037	431.528			
2700	156.900	408.558	243.097	446 747	−1039.325	−428.844	8.296
2800	156.900	414.265	249 109	462.437	−1037.407	−406.268	7.579
2900	156.900	419.770	254.899	478.127	−1035.520	−383.762	6.912
3000	156 900	425.090	260 484	493.817	−1711.697	−352.093	6.130
3100	156.900	430.234	265.877	509.507	−1708.210	−306.830	5.170
3200	156 900	435.216	271.092	525.197	−1704.851	−261.679	4.271
3300	156.900	440 044	276.139	540.887	−1701 615	−216.631	3.429
3400	156.900	444.728	281.029	556.577	−1698 498	−171.678	2.638
3500	156.900	449.276	285.771	572.267	−1695.500	−126.816	1.893
3600	156 900	453.696	290.374	587.957	−1692.618	−82.037	1.190
3700	156.900	457.995	294.847	603.647	−1689.852	−37.338	0.527
3800	156.900	462.179	299.196	619.337	−1687.205	7.291	−0.100
3900	156.900	466.254	303.427	635.027	−1684.678	51.850	−0.694
4000	156.900	470.227	307.548	650.717	−1682.276	96.344	−1.258
4100	156 900	474.101	311.563	666.407	−1680.003	140.782	−1.794
4200	156.900	477.882	315.478	682.097	−1677.867	185.165	−2.303
4300	156.900	481.574	319.298	697.787	−1675.874	229.500	−2.788
4400	156.900	485.181	323.027	713.477	−1674.034	273.788	−3.250
4500	156.900	488.707	326.670	729.167	−1672.356	318.037	−3.692

PREVIOUS. CURRENT: December 1973

Chromium Oxide (Cr_2O_3) $Cr_2O_3(cr,l)$

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Cesium (Cs) **REFERENCE STATE**

$A_r = 132.9054$ **Cesium (Cs)** Cs_1**(ref)**

0 to 301.55 K crystal
301.55 to 947.967 K liquid
above 947.967 K ideal monatomic gas

Refer to the individual tables for details.

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

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−7.717	0.	0.	0.
100	25.812	54.952	110.635	−5.568	0.	0.	0.
200	27.804	73.453	87.892	−2.888	0.	0.	0.
298.15	32.195	85.147	85.147	0.	0.	0.	0.
300	32.355	85.347	85.148	0.060	0.	0.	0.
301.550	32.501	85.514	85.149	0.110	CRYSTAL <--> LIQUID TRANSITION		
301.550	32.393	92.436	85.149	2.197			
400	31.518	101.458	88.110	5.339	0.	0.	0.
500	31.154	108.448	91.506	8.471	0.	0.	0.
600	30.999	114.113	94.817	11.578	0.	0.	0.
700	30.941	118.887	97.923	14.674	0.	0.	0.
800	30.932	123.017	100.808	17.768	0.	0.	0.
900	30.957	126.662	103.482	20.862	0.	0.	0.
947.967	30.976	128.270	104.696	22.348	LIQUID <--> IDEAL GAS FUGACITY = 1 bar		
947.967	20.786	199.643	104.696	90.007			
1000	20.786	200.754	109.665	91.089	0.	0.	0.
1100	20.788	202.735	118.037	93.167	0.	0.	0.
1200	20.791	204.544	125.172	95.246	0.	0.	0.
1300	20.799	206.208	131.342	97.326	0.	0.	0.
1400	20.814	207.750	136.746	99.406	0.	0.	0.
1500	20.841	209.187	141.528	101.489	0.	0.	0.
1600	20.886	210.533	145.799	103.575	0.	0.	0.
1700	20.952	211.802	149.645	105.667	0.	0.	0.
1800	21.048	213.002	153.131	107.767	0.	0.	0.
1900	21.178	214.143	156.313	109.878	0.	0.	0.
2000	21.349	215.233	159.232	112.004	0.	0.	0.
2100	21.564	216.280	161.924	114.149	0.	0.	0.
2200	21.830	217.289	164.417	116.318	0.	0.	0.
2300	22.150	218.266	166.737	118.517	0.	0.	0.
2400	22.527	219.217	168.904	120.750	0.	0.	0.
2500	22.960	220.145	170.935	123.023	0.	0.	0.
2600	23.456	221.055	172.846	125.344	0.	0.	0.
2700	24.016	221.950	174.648	127.717	0.	0.	0.
2800	24.639	222.835	176.353	130.149	0.	0.	0.
2900	25.326	223.711	177.971	132.646	0.	0.	0.
3000	26.082	224.582	179.510	135.216	0.	0.	0.
3100	26.905	225.451	180.978	137.864	0.	0.	0.
3200	27.796	226.319	182.381	140.599	0.	0.	0.
3300	28.599	227.175	183.725	143.384	0.	0.	0.
3400	29.572	228.043	185.016	146.293	0.	0.	0.
3500	30.600	228.915	186.258	149.301	0.	0.	0.
3600	31.680	229.792	187.455	152.414	0.	0.	0.
3700	32.770	230.671	188.610	155.625	0.	0.	0.
3800	33.902	231.557	189.729	158.949	0.	0.	0.
3900	35.036	232.447	190.812	162.375	0.	0.	0.
4000	36.250	233.349	191.864	165.939	0.	0.	0.
4100	37.488	234.259	192.887	169.626	0.	0.	0.
4200	38.744	235.178	193.883	173.438	0.	0.	0.
4300	40.010	236.104	194.854	177.375	0.	0.	0.
4400	40.717	236.965	195.795	181.147	0.	0.	0.
4500	40.901	237.756	196.706	184.728	0.	0.	0.
4600	41.940	238.667	197.608	188.871	0.	0.	0.
4700	42.950	239.580	198.491	193.115	0.	0.	0.
4800	43.924	240.494	199.357	197.459	0.	0.	0.
4900	44.859	241.409	200.206	201.899	0.	0.	0.
5000	45.748	242.325	201.039	206.430	0.	0.	0.
5100	46.588	243.239	201.857	211.047	0.	0.	0.
5200	46.722	244.034	202.647	215.214	0.	0.	0.
5300	47.407	244.931	203.436	219.921	0.	0.	0.
5400	47.729	245.763	204.205	224.415	0.	0.	0.
5500	48.117	246.611	204.964	229.060	0.	0.	0.
5600	48.599	247.483	205.716	233.896	0.	0.	0.
5700	49.022	248.347	206.456	238.778	0.	0.	0.
5800	49.385	249.203	207.186	243.699	0.	0.	0.
5900	49.689	250.049	207.905	248.653	0.	0.	0.
6000	49.935	250.887	208.614	253.634	0.	0.	0.

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