

Cobalt (Co)

A<sub>1</sub> = 58.9332 Cobalt (Co)

REFERENCE STATE

0 to 700.1 K crystal, alpha  
 700.1 to 1768 K crystal, beta  
 1768 to 3184.943 K liquid  
 above 3184.943 K ideal monatomic gas

Refer to the individual tables for details.

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - R ln(T <sub>1</sub> )/T]	Enthalpy Reference Temperature = T <sub>1</sub> = 298.15 K	Standard State Pressure = p <sup>o</sup> = 0.1 MPa		
				H <sup>o</sup> - H <sup>o</sup> (T <sub>1</sub> )	ΔH <sup>o</sup>	log K <sub>f</sub>
0	0	0	INFINITE	-4.771	0	0
100	13.909	7.681	50.176	-4.249	0	0
200	22.226	20.588	32.287	-2.340	0	0
298.15	24.802	30.067	30.067	0	0	0
300	24.833	30.221	30.068	0.046	0	0
400	26.527	37.597	31.062	2.614	0	0
500	28.200	43.700	32.996	5.352	0	0
600	29.665	48.973	35.229	8.246	0	0
700	31.045	53.650	37.533	11.282	0	0
700.100	31.047	53.655	37.535	11.285	ALPHA <- -> BETA	0
700.100	30.583	54.500	37.535	11.757	TRANSITION	0
800	32.426	58.497	39.894	14.883	0	0
900	34.518	62.433	42.181	18.227	0	0
1000	36.987	66.194	44.396	21.799	0	0
1100	39.832	69.849	46.544	25.635	0	0
1200	43.221	73.445	48.636	29.771	0	0
1300	48.660	77.110	50.685	34.354	0	0
1394.000	54.978	80.719	52.587	39.215	C <sub>p</sub> LAMBDA MAXIMUM	0
1394.000	54.999	80.719	52.587	39.215	TRANSITION	0
1400	44.225	80.930	52.708	39.511	0	0
1500	39.748	83.794	54.688	43.659	0	0
1600	38.284	86.307	56.587	47.552	0	0
1700	37.782	88.608	58.404	51.347	0	0
1768.000	37.980	90.092	59.504	53.921	BETA <- -> LIQUID	0
1768.000	40.501	92.251	59.594	70.113	TRANSITION	0
1800	40.501	99.977	60.305	71.409	0	0
1900	40.501	102.167	62.452	75.459	0	0
2000	40.501	104.245	64.490	79.509	0	0
2100	40.501	106.221	66.430	83.560	0	0
2200	40.501	108.105	68.282	87.610	0	0
2300	40.501	109.905	70.053	91.660	0	0
2400	40.501	111.629	71.750	95.710	0	0
2500	40.501	113.282	73.378	99.760	0	0
2600	40.501	114.871	74.944	103.810	0	0
2700	40.501	116.399	76.451	107.860	0	0
2800	40.501	117.872	77.904	111.910	0	0
2900	40.501	119.293	79.307	115.961	0	0
3000	40.501	120.666	80.663	120.011	0	0
3100	40.501	121.994	81.975	124.061	0	0
3184.943	40.501	123.089	83.057	127.501	LIQUID <- -> IDEAL GAS	0
3184.943	26.233	240.840	83.057	502.529	FUGACITY = 1 bar	0
3200	26.233	240.963	83.800	502.924	0	0
3300	26.245	241.771	88.574	505.548	0	0
3400	26.269	242.555	93.092	508.174	0	0
3500	26.305	243.317	97.373	510.802	0	0
3600	26.354	244.058	101.437	513.435	0	0
3700	26.416	244.781	105.502	516.073	0	0
3800	26.491	245.487	109.582	518.719	0	0
3900	26.579	246.176	112.491	521.372	0	0
4000	26.679	246.850	115.841	524.035	0	0
4200	26.919	248.157	122.111	529.394	0	0
4400	27.209	249.416	127.869	534.806	0	0
4600	27.546	250.633	133.180	540.281	0	0
4800	27.930	251.813	138.099	545.827	0	0
5000	28.358	252.962	142.671	551.456	0	0
5200	28.829	254.083	146.934	557.174	0	0
5400	29.342	255.181	150.923	562.990	0	0
5600	29.896	256.258	154.666	568.913	0	0
5800	30.492	257.317	158.187	574.951	0	0
6000	31.003	258.351	161.508	581.056	0	0

PREVIOUS: September 1967 (1 atm)

CURRENT: September 1967 (1 bar)

Cobalt (Co)

Co<sub>1</sub>(ref)

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

## Cobalt (Co)

 $M_r = 58.9332$  Cobalt (Co)Co<sub>1</sub>(cr)

$S^\circ(298.15 \text{ K}) = 30.067 \pm 0.10 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_m(\alpha \rightarrow \beta) = 700 \text{ K}$   
 $T_{fus} = 923 \pm 1 \text{ K}$

$\Delta_f H^\circ(0 \text{ K}) = 0 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = 0 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\alpha\beta} H^\circ = 0.452 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\alpha\beta} H^\circ(923 \text{ K}) = 16.192 \pm 0.25 \text{ kJ}\cdot\text{mol}^{-1}$

## Enthalpy of Formation

Zero by definition.

## Heat Capacity and Entropy

The heat capacity of Co(cr) is adopted from Hultgren *et al.*<sup>1</sup> Their selected values are based on the data from nineteen investigations. The entropy values are based on  $S^\circ(1 \text{ K}) = 0.0011 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . The heat capacity has a maximum value of  $13.14 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  at the Curie point (1394 K).

## Transition Data

The exact nature of the  $\alpha(\text{hcp})$ - $\beta(\text{fcc})$  transition is yet to be clearly elucidated. Three investigations<sup>2-4</sup> indicate that it is not a simple time- and temperature-dependent phenomenon. Crystalline cobalt exists as pure  $\beta$ -phase above 700 K whereas mixtures of alpha and beta cobalt commonly coexist in varying proportions below this temperature. The values of  $T_m$  and  $\Delta_{\alpha\beta} H^\circ$  are those selected by Hultgren *et al.*<sup>1</sup>

## Fusion Data

The temperature and enthalpy of melting are those selected by Hultgren *et al.*<sup>1</sup>

## Sublimation Data

The enthalpy of sublimation is calculated from the data of Edwards *et al.*<sup>5</sup> See the ideal gas table for details.

## References

- <sup>1</sup>R. Hultgren, R. L. Orr and K. K. Kelley, Supplement to Selected Values of Thermodynamic Properties of Metal and Alloys, University of California, Berkeley, Calif., (1966).
- <sup>2</sup>O. S. Edwards and H. Lipson, *J. Inst. Metals* **69**, 177 (1943).
- <sup>3</sup>A. R. Rtoiano and J. L. Tokich, *Trans. Am. Inst. Mining Met. Engrs.* **175**, 728 (1948).
- <sup>4</sup>P. R. Rao, *Proc. Indian Acad. Sci. Sect. A*, **61**, 230 (1965).
- <sup>5</sup>J. W. Edwards, H. L. Johnston and W. E. Dimars, *J. Am. Chem. Soc.* **73**, 4729 (1951).

T/K	C <sub>p</sub> <sup>a</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		
		S <sup>b</sup> / J·K <sup>-1</sup> ·mol <sup>-1</sup>	-(G <sup>o</sup> - FF(T <sub>r</sub> ))/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ) / kJ·mol <sup>-1</sup>	Δ <sub>f</sub> G <sup>o</sup> / kJ·mol <sup>-1</sup>	log K <sub>r</sub>
0	0	0	INFINITE	-4.771	0	0
100	13.909	7.681	50.176	-4.249	0	0
200	22.226	20.588	32.287	-2.240	0	0
250	23.984	25.738	30.475	-1.184	0	0
298.15	24.802	30.067	30.067	0	0	0
300	24.833	30.221	30.068	0.046	0	0
350	25.682	34.113	30.373	1.209	0	0
400	26.577	37.597	31.062	2.614	0	0
450	27.500	40.772	31.807	3.952	0	0
500	28.200	43.700	32.596	5.352	0	0
600	29.665	48.973	35.229	8.246	0	0
700	31.045	53.650	37.533	11.282	0	0
700.100	31.047	53.655	37.535	11.285	ALPHA <- -> BETA TRANSITION	0
700.100	30.583	54.300	37.535	11.737	0	0
800	32.426	58.497	39.894	14.885	0	0
900	34.518	62.453	42.181	18.227	0	0
1000	36.987	66.194	44.596	21.759	0	0
1100	39.832	69.849	46.544	25.635	0	0
1200	43.221	73.445	48.636	29.771	0	0
1300	48.660	77.110	50.685	34.354	0	0
1394.000	54.978	80.719	52.587	39.215	C <sub>p</sub> LAMBDA MAXIMUM TRANSITION	0
1394.000	54.999	80.719	52.587	39.215	0	0
1400	44.225	80.930	52.708	39.511	0	0
1500	39.748	85.794	54.688	43.659	0	0
1600	38.284	86.307	56.587	47.552	0	0
1700	37.782	88.608	58.404	51.347	0	0
1768.000	37.990	90.092	59.594	53.921	BETA <- -> LIQUID TRANSITION	0
1800	37.656	90.776	60.142	55.141	-16.269	0.293
1900	37.656	91.869	61.869	58.906	-16.553	1.221
2000	37.656	94.744	63.408	62.672	-16.858	2.164
2100	37.656	96.581	64.944	66.437	-17.122	3.121
2200	37.656	98.333	66.422	70.203	-17.407	4.092
2300	37.656	100.006	67.846	73.969	-17.691	5.076
2400	37.656	101.609	69.220	77.734	-17.976	6.071
2500	37.656	103.146	70.546	81.500	-18.260	7.079

PREVIOUS:

CURRENT: September 1967

## Cobalt (Co)

Co<sub>1</sub>(cr)

Co<sub>1</sub>(l)

Cobalt (Co)  $M_r = 58.9332$

LIQUID

Cobalt (Co)

$S^\circ(298.15\text{ K}) = [41.000] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = 1768\text{ K}$   
 $\Delta H_f^\circ(298.15\text{ K}) = [18.004] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{vap}}H^\circ = 16.192 \pm 0.25 \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**

The enthalpy of formation is calculated from that of the crystal by adding  $\Delta_{\text{vap}}H^\circ$  and the difference in  $H^\circ(1768\text{ K}) - H^\circ(298.15\text{ K})$ , between the crystal and liquid.

**Heat Capacity and Entropy**

The heat capacity of Co(l) selected by Hulgren *et al.*<sup>1</sup> is used at temperatures above 1768 K. The capacities at temperatures below the melting point are estimated by assuming a glass transition at 1100 K and heat capacities similar to those of the crystal below 1100 K.

**Fusion Data**

Refer to the crystal table for details.

**Vaporization Data**

The boiling point is calculated from the adopted thermodynamic functions and the chosen enthalpy of sublimation at 298.15 K so that the Gibbs energy functions calculated by integration of the crystal liquid data and by statistical methods from the gas phase are equal at the boiling point.

**Reference**

<sup>1</sup>R. Hulgren, R. L. Orr and K. K. Kelley, Supplement to Selected Values of Thermodynamic Properties of Metals and Alloys, University of California, Berkeley, Calif. (1966).

7/K	$C_p^\circ$	$S^\circ - [C_p^\circ - H^\circ(T)]/T$	$H^\circ - H^\circ(T)$	$\Delta_{\text{vap}}H^\circ$	$\Delta_{\text{liq}}G^\circ$	log $K_f$
0	0	0	0	18.004	14.745	-2.583
100	24.811	41.000	41.000	18.004	14.724	-2.564
200	24.842	41.000	0.046	18.004	14.178	-2.564
300	25.686	41.000	1.309	18.004	13.614	-1.780
400	26.527	41.000	2.614	18.005	13.051	-1.819
500	27.390	41.000	3.963	18.005	12.538	-1.310
600	28.200	41.000	5.353	18.005	12.066	-0.996
700	29.665	41.000	6.786	18.006	11.634	-0.772
800	30.878	41.000	8.268	17.994	11.242	-0.609
900	32.426	41.000	9.797	17.994	10.894	-0.481
1000	34.518	41.000	11.369	17.994	10.589	-0.379
1100	36.987	41.000	12.994	17.994	10.326	-0.296
1200	39.832	41.000	14.673	17.994	10.103	---
1300	43.066	41.000	16.406	17.994	9.920	---
1400	46.700	41.000	18.194	17.994	9.777	---
1500	50.734	41.000	20.037	17.994	9.664	---
1600	55.170	41.000	21.935	17.994	9.577	---
1700	60.000	41.000	23.887	17.994	9.511	---
1768.000	64.231	41.000	25.894	17.994	9.462	---
1800	68.864	41.000	27.957	17.994	9.428	---
1900	73.900	41.000	29.977	17.994	9.406	---
2000	79.340	41.000	31.954	17.994	9.393	---
2100	85.176	41.000	33.888	17.994	9.388	---
2200	91.400	41.000	35.779	17.994	9.390	---
2300	98.000	41.000	37.626	17.994	9.397	---
2400	104.976	41.000	39.429	17.994	9.408	---
2500	112.320	41.000	41.188	17.994	9.423	---
2600	120.032	41.000	42.902	17.994	9.441	---
2700	128.104	41.000	44.571	17.994	9.462	---
2800	136.536	41.000	46.195	17.994	9.485	---
2900	145.328	41.000	47.774	17.994	9.511	---
3000	154.480	41.000	49.307	17.994	9.539	---
3100	164.000	41.000	50.794	17.994	9.569	---
3184.943	173.900	41.000	52.235	17.994	9.600	---
3200	174.200	41.000	52.500	17.994	9.605	---
3300	184.943	41.000	54.405	17.994	9.643	---
3400	196.128	41.000	56.266	17.994	9.683	---
3500	207.756	41.000	58.082	17.994	9.724	---
3600	219.828	41.000	59.853	17.994	9.766	---
3700	232.344	41.000	61.579	17.994	9.809	---
3800	245.304	41.000	63.260	17.994	9.853	---
3900	258.708	41.000	64.896	17.994	9.898	---
4000	272.556	41.000	66.487	17.994	9.944	---

PREVIOUS:

CURRENT: September 1967

Cobalt (Co)

Co(l)

Cobalt (Co)

A<sub>1</sub> = 58.9332 Cobalt (Co)

CRYSTAL(α-β)-LIQUID

0 to 700.1 K crystal, alpha  
700.1 to 1768 K crystal, beta  
above 1768 K liquid

Refer to the individual tables for details.

Cobalt (Co)

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature - T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>f</sub>
		S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	ΔH <sup>o</sup>	ΔG <sup>o</sup>	
0	0	INFINITE	0	0	0	0
100	13.909	7.681	50.176	-4.771	0	0
200	22.226	20.588	32.287	-4.249	0	0
250	23.984	25.738	30.475	-2.340	0	0
298.15	24.802	30.067	30.067	0	0	0
300	24.833	30.221	30.068	0.046	0	0
350	25.682	34.113	30.373	1.309	0	0
400	26.527	37.597	31.062	2.614	0	0
450	27.390	40.772	31.967	3.962	0	0
500	28.200	43.700	32.996	5.352	0	0
600	29.665	48.973	35.229	8.246	0	0
700	31.045	53.650	37.533	11.282	0	0
700.100	31.047	53.655	37.535	11.285	ALPHA <-> BETA	
700.100	30.583	54.300	37.535	11.737	TRANSITION	
800	32.426	58.497	39.894	14.883	0	0
900	34.518	62.433	42.181	18.227	0	0
1000	36.987	66.194	44.396	21.799	0	0
1100	39.832	69.849	46.544	25.635	0	0
1200	43.271	73.445	48.636	29.771	0	0
1300	46.660	77.111	50.685	34.354	0	0
1394.000	54.978	80.719	52.587	39.215	C <sub>2</sub> LAMBDA MAXIMUM	
1394.000	54.978	80.719	52.587	39.215	TRANSITION	
1400	44.225	80.930	52.708	39.511	0	0
1500	39.748	83.794	54.688	43.659	0	0
1600	38.284	86.307	56.587	47.552	0	0
1700	37.782	88.608	58.404	51.347	0	0
1768.000	37.990	90.092	59.594	53.921	BETA <-> LIQUID	
1768.000	40.501	99.251	59.594	70.113	TRANSITION	
1800	40.501	99.977	60.305	71.409	0	0
1900	40.501	102.167	62.452	75.459	0	0
2000	40.501	104.244	64.490	79.509	0	0
2100	40.501	106.221	66.430	83.560	0	0
2200	40.501	108.105	68.282	87.610	0	0
2300	40.501	109.905	70.053	91.660	0	0
2400	40.501	111.629	71.750	95.710	0	0
2500	40.501	113.282	73.378	99.760	0	0
2600	40.501	114.871	74.944	103.810	0	0
2700	40.501	116.399	76.451	107.860	0	0
2800	40.501	117.872	77.904	111.910	0	0
2900	40.501	119.293	79.307	115.960	0	0
3000	40.501	120.666	80.663	120.011	0	0
3100	40.501	121.994	81.975	124.061	0	0
3184.943	40.501	123.089	83.057	127.501	--- FUGACITY = 1 bar ---	
3200	40.501	123.280	83.246	128.111	1.773	-0.029
3300	40.501	124.526	84.478	132.161	13.519	-0.214
3400	40.501	125.735	85.673	136.211	23.222	-0.387
3500	40.501	126.910	86.835	140.261	36.883	-0.550
3600	40.501	128.050	87.964	144.311	48.504	-0.704
3700	40.501	129.160	89.063	148.361	58.712	-0.848
3800	40.501	130.240	90.132	152.411	66.307	-0.985
3900	40.501	131.292	91.174	156.462	71.629	-1.113
4000	40.501	132.318	92.190	160.512	74.606	-1.235

PREVIOUS:

CURRENT: September 1967

Cobalt (Co)

Co<sub>1</sub>(cr,l)

Cobalt (Co)

$IP(\text{Co}, g) = 63430 \pm 50 \text{ cm}^{-1}$   
 $S^\circ(298.15 \text{ K}) = 179.52 \pm 0.01 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

IDEAL GAS

Electronic Levels and Quantum Weights	$\epsilon$ , $\text{cm}^{-1}$	g,
State	0	10
$^4F_{7/2}$	816.00	8
$^4F_{5/2}$	1406.84	6
$^4F_{3/2}$	1809.33	4
	.	.
	.	.
$^5H_6$	125969.5	13
IP	63430	

$\Delta_f H^\circ(0 \text{ K}) = 425.1 \pm 2.1 \text{ kJ} \cdot \text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = [426.7] \text{ kJ} \cdot \text{mol}^{-1}$

$A_r = 58.9332$  Cobalt (Co)

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

T/K	C <sub>v</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>v</sub> <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )/T	$\Delta_f H^\circ$	Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$		log K <sub>r</sub>
					$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0	INFINITE	INFINITE	INFINITE	425.087	425.087	INFINITE
100	20.793	156.132	0	-6.360	198.942	215.102	0
200	21.452	170.670	181.570	-2.180	426.836	396.819	-103.639
250	22.214	175.536	179.892	-1.089	426.771	389.322	-81.344
298.15	23.074	179.518	179.518	0	426.676	382.117	-66.945
300	23.054	179.650	179.650	0.043	426.673	381.541	-66.484
350	23.841	183.274	179.802	1.715	426.687	374.376	-53.872
400	24.508	186.503	180.441	2.435	426.784	368.284	-47.915
450	25.034	189.421	181.279	3.664	426.978	363.265	-41.728
500	25.425	192.080	182.229	4.926	427.250	359.280	-36.779
600	25.890	196.762	184.271	7.495	427.924	352.501	-29.360
700	26.323	200.771	186.349	10.095	428.489	347.504	-24.066
800	26.718	204.162	188.375	12.710	428.981	343.891	-20.103
900	27.075	207.350	190.353	15.341	429.411	341.262	-17.026
1000	27.400	210.119	192.159	17.960	429.788	339.213	-14.669
1100	27.699	212.631	193.908	20.596	430.137	337.676	-12.564
1200	27.979	214.932	195.565	23.240	430.459	336.561	-10.898
1300	28.238	217.054	197.138	25.892	430.757	335.787	-9.494
1400	28.479	218.923	198.632	28.551	431.035	335.233	-8.297
1500	28.697	220.684	200.053	31.216	431.288	334.876	-7.265
1600	28.890	222.356	201.408	33.885	431.519	334.682	-6.365
1700	29.061	223.942	202.702	36.556	431.727	334.639	-5.573
1800	29.213	225.453	203.939	39.229	431.912	334.735	-4.879
1900	29.349	226.892	205.125	41.899	432.075	334.869	-4.278
2000	29.472	228.266	206.262	44.567	432.216	335.032	-3.738
2100	29.583	229.584	207.354	47.232	432.335	335.308	-3.252
2200	29.684	230.854	208.405	49.897	432.433	335.686	-2.821
2300	29.777	232.084	209.417	52.567	432.510	336.159	-2.440
2400	29.862	233.271	210.392	55.247	432.567	336.722	-2.109
2500	29.940	234.421	211.334	57.942	432.605	337.378	-1.799
2600	29.999	235.540	212.244	60.664	432.626	338.121	-1.490
2700	30.052	236.635	213.124	63.418	432.631	338.954	-1.195
2800	30.100	237.701	213.976	66.199	432.621	339.875	-0.912
2900	30.143	238.740	214.802	69.014	432.597	340.883	-0.640
3000	30.181	239.756	215.603	71.862	432.561	341.976	-0.381
3100	30.214	240.730	216.380	74.742	432.511	343.152	-0.169
3184.943	30.233	240.840	217.023	75.854	432.485	343.400	0
3300	30.253	241.817	217.586	78.249	432.444	344.725	0
3400	30.268	242.746	218.070	80.820	432.399	346.198	0
3500	30.278	243.631	218.480	83.568	432.351	347.819	0
3600	30.283	244.478	218.819	86.488	432.301	349.487	0
3700	30.284	245.291	219.088	89.580	432.249	351.302	0
3800	30.281	246.070	219.291	92.843	432.195	353.262	0
3900	30.275	246.816	219.430	96.279	432.140	355.369	0
4000	30.267	247.530	219.511	99.888	432.084	357.624	0
4100	30.256	248.211	219.536	103.670	432.026	360.037	0
4200	30.242	248.859	219.508	107.625	431.967	362.611	0
4300	30.225	249.476	219.428	111.753	431.907	365.357	0
4400	30.206	250.063	219.297	116.054	431.846	368.286	0
4500	30.185	250.621	219.118	120.537	431.784	371.409	0
4600	30.161	251.151	218.893	125.202	431.721	374.736	0
4700	30.134	251.652	218.625	130.050	431.657	378.277	0
4800	30.105	252.126	218.318	135.084	431.592	382.043	0
4900	30.073	252.574	217.976	140.307	431.526	386.046	0
5000	30.038	253.000	217.602	145.722	431.460	390.300	0
5100	29.999	253.404	217.199	151.331	431.393	394.829	0
5200	29.957	253.787	216.769	157.137	431.325	400.658	0
5300	29.911	254.149	216.315	163.154	431.257	406.813	0
5400	29.861	254.492	215.838	169.386	431.188	413.320	0
5500	29.808	254.816	215.339	175.838	431.119	420.207	0
5600	29.752	255.123	214.818	182.515	431.050	427.406	0
5700	29.693	255.413	214.278	189.423	430.980	434.950	0
5800	29.631	255.687	213.720	196.568	430.909	442.886	0
5900	29.566	255.946	213.148	203.956	430.837	451.162	0
6000	29.500	256.190	212.566	211.594	430.764	459.730	0

PREVIOUS: September 1967 (1 atm) | CURRENT: September 1967 (1 bar)

Enthalpy of Formation

The enthalpy of formation is the enthalpy of sublimation at 298.15 K. The adopted value is that reported by Edwards *et al.*<sup>1</sup> Their value is used because their vapor pressure measurements for Fe<sup>0</sup> and Cu<sup>0</sup> have proved to be very reliable. The results obtained by Vinnaikein and Tomash<sup>2</sup> are rejected because their vapor pressure data for Fe<sup>0</sup> resulted in a value for the enthalpy of sublimation which was higher than the accepted value [refer to JANAF Fe(g) Table for details]. The remaining vapor pressure data are rejected either because the drift was too large or because there were not enough points. Second and third law analyses of the available vapor pressure data gave the following results, with reaction A corresponding to Co(c) = Co(g) and reaction B corresponding to Co(l) = Co(g).

Source	Reaction	Method	Data Points	$\Delta_f H^\circ(298.15 \text{ K})$ , kcal·mol <sup>-1</sup>	$\Delta_f H^\circ(298.15 \text{ K})$ , kcal·mol <sup>-1</sup>	Drift
Edwards <sup>1</sup>	A	Langmuir	9	101.54	101.54	$\pm 0.4 \pm 0.7$
Korney <sup>3</sup>	A	Knudsen	8*	95.37	95.37	$-2.4 \pm 0.6$
Dancy <sup>6</sup>	B	Langmuir	1	90.51	90.51	—
Ruff <sup>7</sup>	B	Boiling Pt.	1	99.35	99.35	—
Nesmeyanov <sup>8</sup>	A	Knudsen	3	82.4 ± 2.4	82.31	$-0.1 \pm 1.6$
Nesmeyanov <sup>9</sup>	A	Knudsen	12*	91.7 ± 2.4	83.19	$-5.9 \pm 1.7$
Vinnaikein <sup>3</sup>	A	Knudsen	Eqn	103.34	103.34	+0.3

\*One point rejected due to failure of a statistical test.

Heat Capacity and Entropy

The electronic levels are taken from Moore.<sup>10</sup> All observed levels were used but only the first few levels are listed above. Unobserved levels below 20,000 cm<sup>-1</sup> are estimated.

References

- <sup>1</sup>J. W. Edwards, H. L. Johnston and W. E. Dimars, *J. Am. Chem. Soc.* **73**, 4729 (1951).
- <sup>2</sup>J. W. Edwards, H. L. Johnston and W. E. Dimars, *J. Am. Chem. Soc.* **75**, 2467 (1953).
- <sup>3</sup>E. Z. Vinnaikein and Ya. Tomash, *Russ. J. Phys. Chem.* (English Transl.) **35**, 1042 (1961).
- <sup>4</sup>E. Z. Vinnaikein, *Dokl. Akad. Nauk SSSR* **117**, 632 (1957).
- <sup>5</sup>Iu. V. Korney and V. N. Golubkin, *Dokl. Akad. Nauk SSSR* **99**, 565 (1954).
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- <sup>7</sup>O. Ruff and F. Keilig, *Z. Anorg. Chem.* **129**, 321 (1914).
- <sup>8</sup>An. N. Nesmeyanov and D. D. Man, *Dokl. Akad. Nauk SSSR* **123**, 1064 (1959).
- <sup>9</sup>An. N. Nesmeyanov and D. D. Man, *Izv. Akad. Nauk SSSR, Otd. Tekhn. Nauk*, No. 1 (1960).
- <sup>10</sup>C. E. Moore, *U. S. Nat. Bur. Stand. Circ.* **467**, Volume II, (1949).

Cobalt (Co)

Co<sub>l</sub>(g)

Cobalt, Ion (Co<sup>2+</sup>)

IP(Co<sup>2+</sup>, g) = 137795 ± 10 cm<sup>-1</sup>  
S<sup>o</sup>(298.15 K) = 178.346 ± 0.05 J·K<sup>-1</sup>·mol<sup>-1</sup>

IDEAL GAS

Cobalt, Ion (Co<sup>+</sup>)

Co<sup>2+</sup>(g)

M<sub>r</sub> = 58.93265

Δ<sub>f</sub>H<sup>o</sup>(0 K) = 1183.88 ± 1.0 kJ·mol<sup>-1</sup>  
Δ<sub>f</sub>H<sup>o</sup>(298.15 K) = [1191.597] kJ·mol<sup>-1</sup>

Electronic Level and Quantum Weights	g <sub>l</sub>	g <sub>u</sub>
State	ε <sub>l</sub> , cm <sup>-1</sup>	g <sub>l</sub>
3F <sub>4</sub>	0.00	9
3F <sub>3</sub>	950.51	7
3F <sub>2</sub>	1597.32	5
3F <sub>5</sub>	3350.58	9
.	.	.
.	.	.
3H <sub>6</sub>	125969.5	13
IP	137795	

Enthalpy of Formation

Δ<sub>f</sub>H<sup>o</sup>(Co<sup>2+</sup>, g, 0 K) is calculated from Δ<sub>f</sub>H<sup>o</sup>(Co, g, 0 K) using the spectroscopic value of IP(Co) = 63430 ± 10 cm<sup>-1</sup> (758.79 ± 0.12 kJ·mol<sup>-1</sup>) from Sugar and Corliss.<sup>2</sup> The ionization limit is converted from cm<sup>-1</sup> to kJ·mol<sup>-1</sup> using the factor, 1 cm<sup>-1</sup> = 0.01196266 kJ·mol<sup>-1</sup>, which is derived from the 1973 CODATA fundamental constants.<sup>3</sup> Rosenstock *et al.*<sup>4</sup> and Levin and Lias<sup>5</sup> have summarized additional ionization and appearance potential data.

Δ<sub>f</sub>H<sup>o</sup>(Co<sup>2+</sup>, g, 298.15 K) is calculated from Δ<sub>f</sub>H<sup>o</sup>(Co, g, 0 K) by using IP(Co) with JANAF<sup>1</sup> enthalpies, H<sup>o</sup>(0 K)-H<sup>o</sup>(298.15 K), for Co(g), Co<sup>+</sup>(g), and e (ref). Δ<sub>f</sub>H<sup>o</sup>(Co<sup>2+</sup>) differs from a room temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*<sup>4</sup> Δ<sub>f</sub>H<sup>o</sup>(298.15 K) should be changed by -6.197 kJ·mol<sup>-1</sup> 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 Sugar and Corliss,<sup>2</sup> 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 Co<sup>2+</sup>(g), all levels listed by Sugar and Corliss,<sup>2</sup> as well as estimated levels, are used in the calculation. The observed levels are too numerous to list completely. The calculations indicate that for Co<sup>2+</sup>(g), the thermodynamic functions are independent of the estimated missing levels (for n = 3), the cut-off procedure, and the inclusion of n = 7 levels up to 1000 K, the Gibbs energy function showing variations of 0.05% at this temperature. The reported uncertainty in S<sup>o</sup>(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 > 7), and use of different fill and cut-off procedures.<sup>6</sup>

References

- <sup>1</sup>JANAF Thermochemical Tables: Co(g), 9-30-67; e<sup>-</sup>(ref), 3-31-82.
- <sup>2</sup>J. Sugar and C. Corliss, *J. Phys. Chem. Ref. Data* **10**, 1097 (1981).
- <sup>3</sup>E. R. Cohen and B. N. Taylor, *J. Phys. Chem. Ref. Data* **2**, 663 (1973).
- <sup>4</sup>H. M. Rosenstock, K. Draxl *et al.*, *J. Phys. Chem. Ref. Data* **6**, Supp. 1, 783 pp. (1977).
- <sup>5</sup>R. D. Levin and S. G. Lias, *U. S. Natl. Bur. Stand., NSRDS-NBS-71*, 634 pp. (1982).
- <sup>6</sup>J. R. Downey, Jr., The Dow Chemical Company, AFOSR-TR-78-0960, Contract No. F44620-75-1-0048. (1978).

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
		J·K <sup>-1</sup> ·mol <sup>-1</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	Δ <sub>f</sub> H <sup>o</sup>	
0	0	INFINITE	INFINITE	0	1183.879	-199.922
100	20.187	155.255	187.384	-4.213	1141.133	-198.634
200	21.116	169.718	180.541	-2.125	1132.279	-198.983
250	21.635	174.482	178.709	-1.057	1123.609	-146.728
298.15	22.272	178.346	178.346	0	1114.877	-129.406
300	22.297	178.484	178.346	0.041	1105.947	-115.538
350	22.981	181.973	178.620	1.173	1087.940	-94.714
400	23.606	185.083	179.237	2.338	1069.650	-70.810
450	24.133	187.895	180.045	3.532	1051.262	-68.638
500	24.559	190.461	180.961	4.750	1032.662	-68.638
600	25.165	194.996	182.932	7.238	1013.848	-68.638
700	25.585	198.908	184.941	9.777	994.985	-68.638
800	25.946	202.348	186.906	12.544	976.072	-68.638
900	26.267	205.425	188.796	15.562	957.072	-68.638
1000	26.561	208.216	190.601	17.815	938.094	-68.638
1100	27.067	210.777	192.230	20.303	919.101	-68.638
1200	27.485	213.150	193.698	23.050	900.036	-68.638
1300	28.002	215.369	195.211	25.803	880.883	-68.638
1400	28.740	217.469	197.014	28.638	861.922	-68.638
1500	29.883	219.488	198.445	31.564	843.479	-68.638
1600	31.654	221.469	199.822	34.635	824.913	-68.638
1700	34.287	223.462	201.154	37.924	806.202	-68.638
1800	37.581	225.521	202.450	41.528	787.318	-68.638
1900	42.853	227.700	203.721	45.560	768.234	-68.638
2000	48.890	230.047	204.978	50.138	748.977	-68.638
2100	55.916	232.599	206.232	55.371	729.534	-68.638
2200	63.978	235.373	207.487	61.242	709.559	-68.638
2300	73.064	238.374	208.746	68.701	689.476	-68.638
2400	83.120	241.570	210.009	73.804	669.120	-68.638
2500	85.120	244.919	211.395	83.808	648.498	-68.638
2600	90.025	248.358	212.751	92.579	628.626	-68.638
2700	93.179	251.820	214.134	101.155	609.500	-68.638
2800	94.494	255.238	215.541	111.153	591.129	-68.638
2900	94.073	258.552	216.987	120.995	571.740	-68.638
3000	92.159	261.713	218.406	129.919	558.863	-68.638
3100	89.071	264.687	219.832	138.988	546.438	-68.638
3200	85.155	267.455	221.297	147.705	534.438	-68.638
3300	80.724	270.008	222.735	156.002	522.842	-68.638
3400	76.057	272.349	224.160	163.842	511.740	-68.638
3500	71.364	274.486	225.568	171.212	501.191	-68.638
3600	66.801	276.432	226.954	178.119	491.334	-68.638
3700	62.471	278.207	228.316	184.580	482.064	-68.638
3800	58.431	279.814	229.650	190.623	473.353	-68.638
3900	54.728	281.283	230.955	196.279	465.184	-68.638
4000	51.355	282.626	232.231	201.580	457.569	-68.638
4100	48.306	283.856	233.475	206.560	450.498	-68.638
4200	45.568	284.986	234.688	211.251	443.972	-68.638
4300	43.119	286.029	235.870	215.683	437.948	-68.638
4400	40.933	286.995	237.021	219.884	432.466	-68.638
4500	38.985	287.893	238.142	223.878	427.466	-68.638
4600	37.250	288.730	239.233	227.688	422.908	-68.638
4700	35.707	289.514	240.294	231.334	418.841	-68.638
4800	34.332	290.251	241.327	234.835	415.132	-68.638
4900	33.107	290.946	242.333	238.206	411.732	-68.638
5000	32.015	291.604	243.312	241.461	408.599	-68.638
5100	31.040	292.228	244.265	244.613	405.688	-68.638
5200	30.188	292.822	245.193	247.672	402.953	-68.638
5300	29.286	293.390	246.097	250.649	400.354	-68.638
5400	28.686	293.932	246.978	253.552	397.856	-68.638
5500	28.036	294.453	247.837	256.389	395.528	-68.638
5600	27.489	294.953	248.673	259.166	393.341	-68.638
5700	26.978	295.435	249.490	261.889	391.260	-68.638
5800	26.517	295.900	250.286	264.563	389.341	-68.638
5900	26.099	296.350	251.063	267.193	387.543	-68.638
6000	25.721	296.785	251.821	269.784	385.843	-68.638

PREVIOUS: September 1967 (1 atm)

CURRENT: June 1984 (1 bar)

Cobalt, Ion (Co<sup>+</sup>)

Co<sup>2+</sup>(g)

Co<sup>-</sup>(g)

Cobalt, Ion (Co<sup>-</sup>)

IDEAL GAS

Cobalt, Ion (Co<sup>-</sup>)

EA(Co, g) = 0.661 ± 0.010 eV  
 S°(298.15 K) = 178.412 ± 0.005 J·K<sup>-1</sup>·mol<sup>-1</sup>

ΔH<sup>o</sup>(0 K) = 361.31 ± 4.7 kJ·mol<sup>-1</sup>  
 ΔH<sup>o</sup>(298.15 K) = [356.649] kJ·mol<sup>-1</sup>

State	Electronic Levels and Quantum Weights	g <sub>i</sub>
F <sub>4</sub>	0	9
F <sub>2</sub>	910	7
F <sub>2</sub>	1560	5

**Enthalpy of Formation**

ΔH<sup>o</sup>(Co<sup>-</sup>, g, 0 K) is calculated from ΔH<sup>o</sup>(Co, g, 0 K) using the adopted electron affinity of EA(Co) = 0.661 ± 0.010 eV (63.776 ± 0.965 kJ·mol<sup>-1</sup>). This value, recommended by Hotoop and Lineberger<sup>4</sup> is based on a laser photodetachment electron spectroscopy study.<sup>5</sup> Additional information on Co<sup>-</sup>(g) may be obtained in the critical discussions of Hotoop and Lineberger,<sup>2,4</sup> Rosenstock *et al.*,<sup>5</sup> and Massey.<sup>6</sup>

ΔH<sup>o</sup>(Co<sup>-</sup>, g, 298.15 K) is obtained from ΔH<sup>o</sup>(Co, g, 0 K) by using EA(Co) with JANAF<sup>1</sup> enthalpies, F<sup>o</sup>(0 K) - H<sup>o</sup>(298.15 K), or Co<sup>-</sup>(g), Co(g), and e<sup>-</sup> (ref). ΔH<sup>o</sup>(Co<sup>-</sup> → Co + e<sup>-</sup>, 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.*<sup>5</sup> ΔH<sup>o</sup>(298.15 K) should be changed by +6.197 kJ·mol<sup>-1</sup> if it is to be used in the ion convention that excludes the enthalpy of the electron.

**Heat Capacity and Entropy**

The ground state and fine-structure separations for Co<sup>-</sup>(g) have been experimentally determined by Corderman *et al.*<sup>3</sup> Lacking any experimental evidence as to the existence of stable excited states, we assume no stable excited states exist.

**References**

- <sup>1</sup>JANAF Thermochemical Tables: Co(g), 9-30-67; e<sup>-</sup> (ref), 3-31-82.
- <sup>2</sup>H. Hotoop and W. C. Lineberger, *J. Phys. Chem. Ref. Data*, Volume 14, p. 731 (1985).
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- <sup>5</sup>H. M. Rosenstock, K. Draxl *et al.*, *J. Phys. Chem. Ref. Data* **6**, Supp. 1, 783 pp. (1977).
- <sup>6</sup>H. S. W. Massey, "Negative Ions," 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	ΔH <sup>o</sup>	
0	0	INFINITE	-6.307	361.311	
100	20.788	155.256	-4.228		-55.831
200	21.191	169.734	-2.137		318.675
250	21.768	178.777	-1.064		318.440
298.15	22.438	178.412	0		318.440
300	22.465	178.550	0.042	356.649	318.440
350	23.154	182.066	1.182	356.649	318.440
400	23.755	185.198	2.355	356.649	318.440
450	24.233	188.025	3.556	356.649	318.440
500	24.582	190.597	4.777	356.649	318.440
600	24.937	195.117	7.256	356.649	318.440
700	24.966	198.966	9.753	356.649	318.440
800	24.794	202.290	12.242	356.649	318.440
900	24.531	205.195	14.709	356.649	318.440
1000	24.233	207.765	17.147	356.649	318.440
1100	23.932	210.060	19.555	333.902	232.595
1200	23.646	212.130	21.934	330.067	223.552
1300	23.383	214.012	24.285	325.756	214.847
1400	23.144	215.736	26.611	320.846	206.496
1500	22.931	217.326	28.915	316.974	198.467
1600	22.740	218.799	31.198	313.235	190.691
1700	22.571	220.173	33.464	309.627	183.143
1800	22.420	221.458	35.713	306.150	176.101
1900	22.286	222.667	37.948	302.842	169.894
2000	22.166	223.807	40.171	300.674	164.461
2100	22.059	224.886	42.382	298.618	159.866
2200	21.964	225.910	44.583	296.668	155.950
2300	21.878	226.884	46.775	294.822	152.707
2400	21.800	227.814	48.959	293.089	149.135
2500	21.731	228.702	51.135	291.467	145.253
2600	21.668	229.553	53.305	289.953	141.068
2700	21.611	230.370	55.469	288.548	136.584
2800	21.559	231.155	57.627	287.253	131.708
2900	21.511	231.910	59.781	286.068	126.435
3000	21.468	232.639	61.930	284.993	120.768
3100	21.429	233.342	64.074	284.028	114.714
3200	21.392	234.022	66.215	283.173	108.272
3300	21.359	234.680	68.353	282.428	101.444
3400	21.328	235.317	70.487	281.793	94.135
3500	21.300	235.935	72.619	281.268	86.354
3600	21.273	236.534	74.747	280.853	78.101
3700	21.249	237.117	76.873	280.546	69.376
3800	21.227	237.683	78.997	280.344	60.191
3900	21.206	238.234	81.119	280.246	51.544
4000	21.186	238.771	83.238	280.253	43.444
4100	21.168	239.294	85.356	280.366	35.891
4200	21.151	239.804	87.472	280.584	28.884
4300	21.135	240.301	89.589	280.912	22.424
4400	21.120	240.787	91.699	281.354	16.509
4500	21.106	241.262	93.810	281.908	11.244
4600	21.093	241.725	95.920	282.572	6.629
4700	21.080	242.179	98.029	283.344	2.666
4800	21.069	242.622	100.136	284.223	-1.744
4900	21.058	243.057	102.243	285.208	-4.544
5000	21.047	243.482	104.348	286.300	-7.791
5100	21.038	243.899	106.455	287.499	-11.491
5200	21.028	244.307	108.555	288.806	-15.654
5300	21.020	244.708	110.658	290.221	-20.291
5400	21.011	245.100	112.759	291.744	-25.414
5500	21.004	245.486	114.860	293.374	-31.044
5600	20.996	245.864	116.960	295.109	-37.291
5700	20.989	246.236	119.059	296.949	-44.154
5800	20.982	246.601	121.158	298.894	-51.634
5900	20.976	246.959	123.256	300.944	-59.744
6000	20.970	247.312	125.353	303.099	-68.484

PREVIOUS:

CURRENT: June 1984 (1 bar)

Cobalt, Ion (Co<sup>-</sup>)

Co<sup>-</sup>(g)

Cobalt Fluoride (CoF<sub>2</sub>)

## CRYSTAL

M<sub>r</sub> = 96.930006Cobalt Fluoride (CoF<sub>2</sub>)Co<sub>2</sub>F<sub>3</sub>(cr)

S°(298.15 K) = 82.026 ± 0.42 J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>lim</sub> = 1400 ± 7.0 K  
 $\Delta H_f^\circ(0 \text{ K}) = -670.4 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta H_f^\circ(298.15 \text{ K}) = -671.53 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{sub}}H^\circ = 58.819 \pm 12.6 \text{ kJ}\cdot\text{mol}^{-1}$

## Enthalpy of Formation

Heus and Egan<sup>1</sup> measured the emf of a solid state galvanic cell which involved the reactions: Al(cr) + 3/2 CoF<sub>2</sub>(cr) → AlF<sub>3</sub>(cr) + 3/2 Co(cr), E(873 K) = 1.611 volts; Mg(cr) + CoF<sub>2</sub>(cr) → MgF<sub>2</sub>(cr) + Co(cr), E(873 K) = 2.231 volts. Combining these results with auxiliary thermodynamic data<sup>2</sup> for the reactants and products, we derive  $\Delta H_f^\circ(\text{CoF}_2, \text{cr}, 298.15 \text{ K}) = -160.2$  and  $-159.95 \text{ kcal}\cdot\text{mol}^{-1}$ .

Several equilibrium studies<sup>3-5</sup> involving CoF<sub>2</sub>(cr) have been reported in the literature. 2nd and 3rd law analyses of these equilibrium data are summarized below, auxiliary data for CoO(cr) and CoCl<sub>2</sub>(cr) are from.<sup>6</sup>

Source	Reaction	T/K	Data Points	$\Delta H_f^\circ(298.15 \text{ K})$ , kcal·mol <sup>-1</sup>	3rd law	Drift	* $\Delta H_f^\circ(298.15 \text{ K})$ , kcal·mol <sup>-1</sup>
3	CoF <sub>2</sub> (cr) + 2HCl(g) → CoCl <sub>2</sub> (cr) + 2HF(g)	588-805	3	4.1	1.75 ± 0.4	-1.7 ± 0.1	-162.6 ± 2.0
4	CoF <sub>2</sub> (cr) + H <sub>2</sub> (g) → Co(cr) + 2HF(g)	673-873	3	35.2	31.5 ± 1.0	-4.2 ± 3.5	-161.8 ± 2.0
5	CoF <sub>2</sub> (cr) + H <sub>2</sub> O(g) → CoO(cr) + 2HF(g)	773-1023	5	30.2	31.1 ± 0.2	0.9 ± 0.3	-160.45 ± 1.0

\*3rd law values except for the first reaction.

We note that Heus and Egan,<sup>1</sup> in the same paper, measured  $\Delta H_f^\circ(\text{AlF}_3, \text{cr}, 298.15 \text{ K}) = -360.2 \text{ kcal}\cdot\text{mol}^{-1}$ , which is in excellent agreement with the JANAF value.<sup>2</sup> Domange<sup>3</sup> also measured similar equilibria for MgF<sub>2</sub> and CaF<sub>2</sub>, which were very consistent with the JANAF enthalpies of formation.<sup>2</sup> Jellinek and Rudat<sup>4</sup> reported similar equilibria for PbF<sub>2</sub>(cr), which show excellent consistency with the JANAF enthalpy of formation.<sup>2</sup> Thus, it is apparent that these three sets are probably quite reliable, and we adopt  $\Delta H_f^\circ(\text{CoF}_2, \text{cr}, 298.15 \text{ K}) = -160.5 \pm 1 \text{ kcal}\cdot\text{mol}^{-1}$  ( $-671.532 \pm 4.2 \text{ kJ}\cdot\text{mol}^{-1}$ ).

## Heat Capacity and Entropy

Catalano and Stout<sup>7</sup> measured low temperature heat capacities in the temperature range 10 to 300 K. Heat capacity data above 300 K are calculated from the high temperature (468-1400 K) enthalpy data of Binford *et al.*<sup>8</sup> Both sets of data were smoothed by computer and joined at 298.15 K.

The value of S°(298.15 K) is obtained from the low temperature heat capacity data of Catalano and Stout<sup>7</sup> and is based on S°(10 K) = 0.013 cal·K<sup>-1</sup>·mol<sup>-1</sup> (0.05439 J·K<sup>-1</sup>·mol<sup>-1</sup>).

## Fusion Data

Refer to the liquid table for details.

## Sublimation Data

Kana'an *et al.*<sup>9</sup> made sublimation studies of CoF<sub>2</sub> using Knudsen and Langmuir techniques over the temperature range 972-1241 K. 2nd and 3rd law analyses of these sublimation pressures are summarized below.

Method	T/K	Data Points	$\Delta_{\text{sub}}H^\circ(298.15 \text{ K})$ , kcal·mol <sup>-1</sup>	Drift
Knudsen	1058-1242	17	75.0	75.1 ± 0.1
Langmuir	972-1032	8	72.8	75.5 ± 0.2

The selected value is  $\Delta_{\text{sub}}H^\circ(298.15 \text{ K}) = 75.3 \pm 3.0 \text{ kcal}\cdot\text{mol}^{-1}$  (315.055 ± 12.6 kJ·mol<sup>-1</sup>).

## References

- R. J. Heus and J. J. Egan, *Z. Phys. Chem.* **49**, 38 (1966).
- JANAF Thermochemical Tables: AlF<sub>3</sub>(cr), 6-30-70; MgF<sub>2</sub>(cr), 3-31-66; PbF<sub>2</sub>(cr), 6-30-69; CaF<sub>2</sub>(cr), 12-31-68.
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T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K			Standard State Pressure = p° = 0.1 MPa		
	C <sub>p</sub> <sup>o</sup>	S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	Δ <sub>r</sub> H°	ΔG°	log K <sub>r</sub>
0	0	0	INFINITE	-670.395	-670.395	INFINITE
100	33.492	25.002	134.603	-672.334	-657.029	343.197
200	37.584	36.746	87.999	-672.454	-641.555	167.557
298.15	68.909	82.026	82.026	-671.532	-626.562	109.771
300	69.041	82.453	82.028	-671.508	-626.283	109.046
400	75.714	103.350	84.831	-670.016	-611.424	79.844
500	78.927	120.625	90.315	-668.372	-596.565	62.365
600	80.789	135.193	96.613	-666.746	-582.837	50.741
700	82.015	147.744	103.041	-665.190	-568.977	42.458
800	82.902	158.736	109.531	-664.157	-555.271	36.255
900	83.592	168.562	115.378	-662.874	-541.742	31.442
1000	84.161	177.400	121.145	-661.698	-528.551	27.598
1100	84.646	185.444	126.631	-660.813	-515.062	24.438
1200	85.077	192.828	131.844	-660.208	-501.845	21.845
1300	85.475	199.654	136.801	-660.032	-488.654	19.634
1400	85.839	206.002	141.519	-660.415	-475.460	17.740
1400.000	85.839	206.002	141.519	90.276	--> CRYSTAL <--> LIQUID	--> -->
1500	86.186	211.936	146.018	-659.771	-462.269	16.098
1600	86.517	217.509	150.314	-658.858	-449.131	14.663
1700	86.831	222.764	154.423	-657.832	-436.054	13.398
1800	87.140	227.736	158.359	-657.055	-422.744	12.268
1900	87.441	232.455	162.135	-656.507	-408.860	11.240
2000	87.734	236.948	165.765	-656.140	-395.019	10.317

PREVIOUS:

CURRENT: June 1970

Cobalt Fluoride (CoF<sub>2</sub>)Co<sub>2</sub>F<sub>3</sub>(cr)



Co<sub>1</sub>F<sub>2</sub>(l)

M<sub>r</sub> = 96.930006 Cobalt Fluoride (CoF<sub>2</sub>)

LIQUID

Cobalt Fluoride (CoF<sub>2</sub>)

S°(298.15 K) = [86.238] J·K<sup>-1</sup>·mol<sup>-1</sup>  
T<sub>fus</sub> = 1400 ± 7.0 K

Δ<sub>l</sub>H°(298.15 K) = [-637.691] kJ·mol<sup>-1</sup>  
Δ<sub>sub</sub>H° = 58.819 ± 12.6 kJ·mol<sup>-1</sup>

**Enthalpy of Formation**

Δ<sub>l</sub>H°(CoF<sub>2</sub>, l, 298.15 K) is calculated from Δ<sub>l</sub>H°(CoF<sub>2</sub>, cr, 298.15 K) by adding the enthalpy of fusion the difference in enthalpy, H°(1400 K)-H°(298.15), between the crystal and liquid.

**Heat Capacity and Entropy**

The heat capacity of liquid CoF<sub>2</sub> is estimated by comparison with those for FeCl<sub>2</sub>(l), MgF<sub>2</sub>(l), and PbF<sub>2</sub>(l) and is assumed constant in the temperature range 298-3000 K. Binford *et al.*, reported C<sub>p</sub> = 30.3 cal·K<sup>-1</sup>·mol<sup>-1</sup> for liquid CoF<sub>2</sub> at 1444 K. This value is based on only two enthalpy points near the melting point and appears high in comparison with heat capacities for other liquid metal dihalides. Therefore, the value is not adopted.

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

**Fusion Data**

T<sub>fus</sub> = 1400 K is from the high temperature enthalpy studies of Binford *et al.*, Δ<sub>l</sub>H° is calculated from their enthalpy data. Premelting of the sample is assumed to be responsible for the rapid rise in enthalpy near the melting point. This enthalpy is included in Δ<sub>sub</sub>H°.

**Vaporization Data**

T<sub>vap</sub> is the temperature at which the Gibbs energy change for the process CoF<sub>2</sub>(l) → CoF<sub>2</sub>(g) equals zero. The difference between the enthalpy of formation of the gas and liquid at T<sub>vap</sub> is Δ<sub>vap</sub>H°.

**Reference**

J. S. Bindford, Jr., J. M. Strohmenger, and T. H. Hebert, *J. Phys. Chem.*, **71**, 2404 (1967).

T/K	C <sub>p</sub> <sup>o</sup>	S°	S° - [C° - H°(T)]/T	H° - H°(T)	Δ <sub>l</sub> H°	log K <sub>r</sub>
Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		J·K <sup>-1</sup> ·mol <sup>-1</sup>		kJ·mol <sup>-1</sup>		
0				0.		
100	104.600	86.238	86.238		-637.691	104.062
200	104.600	86.885	86.240	0.194	-637.602	103.373
300	104.600	86.976	90.343	10.654	-632.929	75.712
400	104.600	140.317	98.090	21.114	-628.573	59.235
500	104.600	159.388	106.765	31.574	-624.480	48.325
600	104.600	175.312	113.464	42.034	-620.608	40.581
700	104.600	189.480	123.865	52.494	-617.358	34.805
800	104.600	201.800	131.851	62.954	-613.896	30.338
900	104.600	212.820	139.407	73.414	-610.698	26.784
1000	104.600	222.790	146.541	83.874	-607.794	23.891
1200	104.600	231.891	153.280	94.334	-605.216	21.491
1300	104.600	240.264	159.653	104.794	-603.108	19.468
1400	104.600	248.015	165.691	115.254	-601.596	17.740
1400.000	104.600	248.015	165.691	115.254	--- CRYSTAL < -> LIQUID	---
1500	104.600	255.232	171.423	125.714	-599.094	16.246
1600	104.600	261.983	176.874	136.174	-596.356	14.945
1700	104.600	268.324	182.069	146.634	-593.537	13.803
1800	104.600	274.303	187.029	157.094	-606.999	12.783
1900	104.600	279.958	191.772	167.554	-604.461	11.858
2000	104.600	285.324	196.317	178.014	-601.932	11.029
2100	104.600	290.427	200.678	188.474	-599.409	10.282
2200	104.600	295.293	204.869	198.934	-596.889	9.606
2300	104.600	299.943	208.902	209.394	-594.367	8.991
2400	104.600	304.394	212.789	219.854	-591.840	8.429
2500	104.600	308.664	216.539	230.314	-589.305	7.915
2600	104.600	312.767	220.162	240.774	-586.757	7.443
2700	104.600	316.714	223.665	251.234	-584.191	7.007
2800	104.600	320.519	227.057	261.694	-581.612	6.604
2900	104.600	324.189	230.343	272.154	-579.007	6.231
3000	104.600	327.735	233.531	282.614	-576.379	5.884

PREVIOUS:

CURRENT: June, 1970

Cobalt Fluoride (CoF<sub>2</sub>)

Co<sub>1</sub>F<sub>2</sub>(l)

Cobalt Fluoride (CoF<sub>2</sub>)

M<sub>r</sub> = 96.930006 Cobalt Fluoride (CoF<sub>2</sub>)

Co<sub>1</sub>F<sub>2</sub>(cr,l)

0 to 1400 K crystal  
above 1400 K liquid

Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>	
	C <sub>p</sub> <sup>o</sup>	S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	ΔH°		ΔG°
0	0	0	INFINITE	-670.395	-670.395	INFINITE
100	33.492	23.002	134.693	-10.969	-657.099	343.197
200	57.584	56.746	87.999	-6.250	-641.533	167.537
298.15	68.909	82.026	82.026	0	-626.562	109.771
300	69.041	82.453	82.028	0.128	-626.283	109.046
400	75.714	103.350	84.831	7.408	-611.424	70.844
500	78.927	120.625	90.315	15.155	-596.965	62.365
600	80.789	135.193	96.613	23.148	-582.837	50.741
700	82.015	147.744	103.041	31.292	-568.190	42.458
800	82.902	158.756	109.331	39.540	-555.271	36.255
900	83.592	168.562	115.378	47.866	-541.742	31.442
1000	84.161	177.400	121.145	56.254	-528.351	27.598
1100	84.646	185.444	126.631	64.695	-515.062	24.458
1200	85.077	192.828	131.844	73.182	-502.208	21.845
1300	85.475	199.654	136.801	81.710	-488.654	19.634
1400	85.839	206.002	141.519	90.276	-475.460	17.740
1400.000	85.839	206.002	141.519	90.276	-475.460	17.740
1400.000	104.600	248.015	141.519	149.094	CRYSTAL → LIQUID TRANSITION	---
1500	104.600	255.232	148.862	159.554	-599.094	-665.535
1600	104.600	261.983	155.724	170.014	-596.356	-657.786
1700	104.600	268.324	162.163	180.474	-593.537	-649.212
1800	104.600	274.303	168.228	190.934	-606.999	-640.510
1900	104.600	279.958	173.961	201.394	-604.461	-631.330
2000	104.600	285.324	179.396	211.854	-601.932	-622.283
2100	104.600	290.427	184.563	222.314	-599.409	-613.363
2200	104.600	295.293	189.487	232.774	-596.889	-604.562
2300	104.600	299.943	194.189	243.234	-594.367	-595.870
2400	104.600	304.394	198.688	253.694	-591.840	-587.301
2500	104.600	308.664	203.003	264.154	-589.305	-578.850
2600	104.600	312.767	207.146	274.614	-586.757	-570.461
2700	104.600	316.714	211.131	285.074	-584.194	-562.191
2800	104.600	320.519	214.971	295.534	-581.612	-554.016
2900	104.600	324.189	218.674	305.994	-579.007	-545.933
3000	104.600	327.735	222.250	316.454	-576.379	-537.941

PREVIOUS:

CURRENT: June 1970

Cobalt Fluoride (CoF<sub>2</sub>)

Co<sub>1</sub>F<sub>2</sub>(cr,l)

Cobalt Fluoride (CoF<sub>2</sub>)

M<sub>r</sub> = 96.930006 Cobalt Fluoride (CoF<sub>2</sub>)

IDEAL GAS

Cobalt Fluoride (CoF<sub>2</sub>)

$\Delta_f H^\circ(0\text{ K}) = -355.82 \pm 12.6\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = -356.48 \pm 12.6\text{ kJ}\cdot\text{mol}^{-1}$

$S^\circ(298.15\text{ K}) = 278.04 \pm 12.6\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

Electronic Levels and Quantum Weights	$g_i$
State	$\epsilon_i, \text{cm}^{-1}$
$^4\Sigma$	0
	[300]
	[4000]
	[9000]

Vibrational Frequencies and Degeneracies	$\nu_i, \text{cm}^{-1}$
	[600](1)
	[151](1)
	762 (1)

$\sigma = 2$

Point Group: C<sub>2v</sub>

Bond Distance: Co-F = [1.72] Å

Bond Angle: F-Co-F = [165]°

Product of Moments of Inertia:  $I_A I_B I_C = 6.57815 \times 10^{-116}\text{ g}^3\cdot\text{cm}^6$

Enthalpy of Formation

$\Delta_f H^\circ(\text{CoF}_2, g, 298.15\text{ K}) = -85.2 \pm 3.0\text{ kcal}\cdot\text{mol}^{-1}$  ( $-355.477 \pm 12.6\text{ kJ}\cdot\text{mol}^{-1}$ ), is calculated from the enthalpy of formation of the crystal,  $\Delta_f H^\circ(\text{CoF}_2, cr, 298.15\text{ K}) = -160.5 \pm 4.0\text{ kcal}\cdot\text{mol}^{-1}$ , and the enthalpy of sublimation,  $\Delta_{sub} H^\circ(298.15\text{ K}) = 75.3 \pm 3.0\text{ kcal}\cdot\text{mol}^{-1}$ . The sublimation value is determined from a 3rd law analysis of the vapor pressure data for CoF<sub>2</sub> reported by Kana *et al.*<sup>1</sup> Refer to the crystal table for details.

Heat Capacity and Entropy

Buchler *et al.*<sup>2</sup> investigated the deflection of a molecular beam of CoF<sub>2</sub>(g) by an electric field and found that within the sensitivity of the apparatus the molecule was nonpolar and consequently possessed a linear structure. Hastie *et al.*<sup>3</sup> recently investigated the infrared absorption spectra of several transition metal difluorides through the use of matrix isolation techniques. Isotopic shift measurements for matrix isolated NiF<sub>2</sub>, ZnF<sub>2</sub>, and CuF<sub>2</sub> in neon and argon indicated that these species were slightly bent. Based upon these results, the authors estimated the F-Co-F angle as 165°. This value is adopted here. The bond length was estimated by Brewer *et al.*<sup>4</sup> The principal moments of inertia are:  $I_A = 0.1934 \times 10^{-39}$ ,  $I_B = 18.3484 \times 10^{-39}$ , and  $I_C = 18.5417 \times 10^{-39}\text{ g}\cdot\text{cm}^2$ .

Hastie *et al.*<sup>3</sup> isolated CoF<sub>2</sub> in neon and argon matrices and observed the  $\nu_2$  fundamental at  $762\text{ cm}^{-1}$ . They also calculated  $\nu_1 = 600\text{ cm}^{-1}$  by a valence force field method and estimated  $\nu_3$  as  $151\text{ cm}^{-1}$  by applying the variation in the frequencies for the chlorides of Co, Ni, Cu, and Zn to the fluorides. The electronic levels and quantum weights are estimated by comparison with the electronic energy levels for Co<sup>2+</sup>(g) ion<sup>5</sup> and those for CoCl<sub>2</sub>(g) observed by Houghen *et al.*<sup>6</sup>

References

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T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - [C <sub>p</sub> <sup>o</sup> - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	Δ <sub>f</sub> G°	
0	0	0	INFINITE	-355.821	INFINITE
100	41.091	227.574	320.907	-350.595	188.355
200	47.569	282.621	486.21	-345.424	95.439
250	49.634	269.160	278.877	-357.752	76.838
298.15	51.210	278.042	278.042	-369.949	64.813
300	51.263	278.359	278.043	-366.486	64.428
350	52.366	286.361	278.672	-356.741	55.558
400	53.288	293.444	280.084	-347.470	48.901
450	54.305	299.795	281.928	-337.632	43.718
500	54.920	305.550	284.007	-327.500	39.568
600	55.822	315.648	288.462	-318.892	33.334
700	56.459	324.303	292.979	-312.500	28.869
800	56.956	331.876	297.377	-308.652	25.507
900	57.377	338.609	301.591	-306.279	22.883
1000	57.753	344.674	305.601	-304.975	20.776
1100	58.095	350.195	309.408	-304.062	19.045
1200	58.410	355.263	313.021	-303.464	17.594
1300	58.699	359.950	316.453	-303.147	16.359
1400	58.964	364.310	319.718	-303.005	15.293
1500	59.205	368.387	322.828	-303.255	14.362
1600	59.424	372.215	325.796	-303.704	13.543
1700	59.623	375.823	328.634	-304.375	12.818
1800	59.801	379.256	331.351	-305.268	12.161
1900	59.963	382.494	333.957	-306.381	11.554
2000	60.108	385.554	336.461	-307.715	11.005
2100	60.239	388.489	338.869	-309.265	10.505
2200	60.356	391.295	341.189	-311.035	10.049
2300	60.461	393.980	343.426	-313.027	9.631
2400	60.555	396.555	345.586	-315.240	9.246
2500	60.638	399.029	347.675	-317.675	8.889
2600	60.712	401.409	349.696	-320.342	8.559
2700	60.777	403.701	351.654	-323.257	8.252
2800	60.834	405.912	353.553	-326.433	7.966
2900	60.882	408.048	355.295	-329.882	7.698
3000	60.924	410.113	356.924	-333.625	7.447
3100	60.959	412.111	358.451	-337.675	7.211
3200	60.988	414.047	360.000	-342.045	6.986
3300	61.011	415.924	362.265	-346.745	6.781
3400	61.029	417.746	364.870	-351.785	6.594
3500	61.041	419.515	367.335	-357.175	6.434
3600	61.050	421.235	369.691	-362.925	6.291
3700	61.054	422.907	371.940	-369.056	6.163
3800	61.054	424.536	374.095	-375.575	6.049
3900	61.051	426.121	376.157	-382.495	5.948
4000	61.044	427.667	378.125	-389.825	5.856
4100	61.035	429.174	379.999	-397.575	5.772
4200	61.023	430.645	381.774	-405.745	5.695
4300	61.009	432.081	383.451	-414.335	5.628
4400	60.992	433.483	385.028	-423.355	5.568
4500	60.973	434.853	386.505	-432.815	5.514
4600	60.953	436.193	387.882	-442.725	5.464
4700	60.931	437.504	389.161	-453.085	5.419
4800	60.908	438.787	390.344	-463.905	5.378
4900	60.883	440.042	391.431	-475.185	5.340
5000	60.858	441.272	392.424	-486.925	5.306
5100	60.831	442.477	393.323	-499.135	5.276
5200	60.804	443.658	394.128	-511.815	5.249
5300	60.776	444.816	394.841	-524.965	5.224
5400	60.747	445.951	395.464	-538.585	5.201
5500	60.718	447.066	396.000	-552.675	5.179
5600	60.689	448.160	396.451	-567.235	5.159
5700	60.659	449.234	396.818	-582.265	5.140
5800	60.629	450.288	397.101	-597.765	5.123
5900	60.599	451.324	397.324	-613.735	5.108
6000	60.569	452.343	397.498	-630.175	5.094

PREVIOUS, June 1970 (1 atm)

CURRENT, June 1970 (1 bar)

Co<sub>2</sub>F<sub>2</sub>(g)

Cobalt Fluoride (CoF<sub>2</sub>)

Cobalt Fluoride (CoF<sub>3</sub>)

## CRYSTAL

$$M_r = 115.928409$$

$S^\circ(298.15 \text{ K}) = 194.6 \pm 12.6 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$   
 $T_{\text{fus}} = [1200 \pm 200] \text{ K}$   
 $\Delta_f H^\circ(0 \text{ K}) = \text{Unknown}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = -790.36 \pm 12.6 \text{ kJ} \cdot \text{mol}^{-1}$   
 $\Delta_{\text{red}} H^\circ = \text{Unknown}$

## Enthalpy of Formation

Fowler *et al.*<sup>1</sup> determined calorimetrically the enthalpy of fluorination of crystalline CoF<sub>2</sub> at 473.15 K. For the reaction  $2 \text{CoF}_2(\text{cr}) + \text{F}_2(\text{g}) \rightarrow \text{CoF}_3(\text{cr})$  they reported  $\Delta_f H^\circ(473.15 \text{ K}) = -52.0 \pm 3.0 \text{ kcal} \cdot \text{mol}^{-1}$  which yields  $\Delta_f H^\circ(298.15 \text{ K}) = -52.4 \pm 3.0 \text{ kcal} \cdot \text{mol}^{-1}$  based upon our functions for CoF<sub>2</sub>(cr) and CoF<sub>3</sub>(cr). Combining this result with the enthalpy of formation of CoF<sub>2</sub>(cr),<sup>2</sup> we derive  $\Delta_f H^\circ(\text{CoF}_3, \text{cr}, 298.15 \text{ K}) = -186.7 \pm 3.0 \text{ kcal} \cdot \text{mol}^{-1}$ .

Jessup *et al.*<sup>3</sup> investigated calorimetrically this same fluorination reaction and reported  $\Delta_f H^\circ(523.15 \text{ K}) = -56.1 \pm 2.0 \text{ kcal} \cdot \text{mol}^{-1}$ . This result leads to  $\Delta_f H^\circ(\text{CoF}_3, \text{cr}, 298.15 \text{ K}) = -188.8 \pm 2.0 \text{ kcal} \cdot \text{mol}^{-1}$ . In the same investigation Jessup *et al.*<sup>3</sup> reported  $\Delta_f H^\circ(608 \text{ K}) = -74.0 \pm 4.0 \text{ kcal} \cdot \text{mol}^{-1}$  for the reduction reaction  $2 \text{CoF}_3(\text{cr}) + \text{H}_2(\text{g}) \rightarrow 2 \text{CoF}_2(\text{cr}) + 2 \text{HF}(\text{g})$ . Corrected to 298.15 K we calculate  $\Delta_f H^\circ(298.15 \text{ K}) = -73.3 \pm 4.0 \text{ kcal} \cdot \text{mol}^{-1}$ . Combining this result with enthalpy of formation data for CoF<sub>2</sub>(cr),<sup>2</sup> and HF(g),<sup>4</sup> we derive  $\Delta_f H^\circ(\text{CoF}_3, \text{cr}, 298.15 \text{ K}) = -189.0 \pm 4.0 \text{ kcal} \cdot \text{mol}^{-1}$ . We note that the addition of these two results by Jessup *et al.*<sup>3</sup> leads to  $\Delta_f H^\circ(298.15 \text{ K}) = -129.9 \pm 6.0 \text{ kcal} \cdot \text{mol}^{-1}$  for the reaction  $\text{H}_2(\text{g}) + \text{F}_2(\text{g}) \rightarrow 2 \text{HF}(\text{g})$  which is quite consistent with the result  $-130.28 \pm 0.4 \text{ kcal} \cdot \text{mol}^{-1}$  calculated from the selected value for the enthalpy of formation of HF(g).<sup>4</sup> Thus, it is apparent that these two results are probably quite reliable, and we adopted  $\Delta_f H^\circ(\text{CoF}_3, \text{cr}, 298.15 \text{ K}) = -188.9 \pm 3.0 \text{ kcal} \cdot \text{mol}^{-1}$  ( $-790.358 \pm 12.6 \text{ kJ} \cdot \text{mol}^{-1}$ ).

Jellinek and Koop<sup>5</sup> reported equilibrium constants for the reduction reaction given above in the temperature range 470–595 K. 2nd and 3rd law analyses of these equilibrium data give  $\Delta_f H^\circ(298.15 \text{ K})$  of 31.7 and 29.3  $\pm 0.6 \text{ kcal} \cdot \text{mol}^{-1}$ , respectively; the drift is  $-4.7 \pm 1.5 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ . These values are in considerable disagreement with the calorimetric value of  $-73.3 \pm 4.0 \text{ kcal} \cdot \text{mol}^{-1}$  given by Jessup *et al.* [3], and no weight is given to these equilibrium data.

## Heat Capacity and Entropy

Heat capacity data for CoF<sub>3</sub>(cr) are estimated by comparison with those for FeF<sub>2</sub>(cr), FeF<sub>3</sub>(cr), TiF<sub>3</sub>(cr), and CoF<sub>2</sub>(cr).  $S^\circ(298.15 \text{ K})$  is estimated to be  $22.6 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  ( $94.5384 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ ) from the ionic entropy contributions given by Kubaschewski, Evans, and Alcock.<sup>6</sup> We note that this method leads to  $S^\circ(298.15 \text{ K}) = 19.4 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  for CoF<sub>2</sub>(cr) which is in good agreement with the experimental value of  $19.60 \pm 0.10 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ .

## Fusion Data

$T_{\text{fus}}$  is estimated by comparison with those for other transition metal halides. We note that Ruff and Ascher<sup>7</sup> reported CoF<sub>3</sub>(cr) being thermally unstable around 900 K, while Stewart<sup>8</sup> recently showed that CoF<sub>3</sub>(cr) was formed by hydrolytic reactions and not by thermal decomposition. The derived  $\Delta_f G^\circ$  values for CoF<sub>3</sub>(cr) indicate that it is thermodynamically more stable than CoF<sub>2</sub>(cr) in agreement with the findings of Stewart.<sup>8</sup> In the temperature range 298–900 K, the Gibbs energy change for the decomposition reaction  $2 \text{CoF}_3(\text{cr}) \rightarrow 2 \text{CoF}_2(\text{cr}) + \text{F}_2(\text{g})$  are in the range  $+10$ – $20 \text{ kcal} \cdot \text{mol}^{-1}$ .

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Cobalt Fluoride (CoF<sub>3</sub>)Co<sub>2</sub>F<sub>3</sub>(cr)

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>i</sub>
		S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )/T	Δ <sub>f</sub> H <sup>o</sup>	Δ <sub>f</sub> G <sup>o</sup>	
0						
100		94.558	0	-790.358	-718.893	125.947
200		95.128	94.560	-790.320	-718.450	125.093
298.15	91.797	122.481	98.255	-788.197	-694.811	90.733
300	92.471	105.375	105.375	-786.113	-671.708	70.173
400	97.470	144.498	144.498	-784.209	-649.010	56.501
600	100.454	162.742	162.742	-782.489	-626.614	46.759
700	101.219	178.285	178.285	-781.344	-604.393	39.463
800	101.981	191.849	191.849	-779.930	-582.361	33.799
900	102.839	203.909	203.909	-778.703	-560.477	29.276
1000	103.868	214.796	214.796	-777.675	-538.706	25.581
1100	105.027	224.750	224.750	-776.867	-517.019	22.505
1200	106.248	233.940	233.940	-776.212	-495.386	19.205
1300	107.587	242.497	242.497	-775.699	-473.771	15.777
1400	108.935	250.519	250.519	-775.330	-452.188	
1500	110.320	258.082	258.082			

PREVIOUS:

CURRENT: December 1970

Cobalt Fluoride (CoF<sub>3</sub>)Co<sub>2</sub>F<sub>3</sub>(cr)

Co<sub>3</sub>O<sub>4</sub>(cr)

M<sub>r</sub> = 74.9326 Cobalt Oxide (CoO)

CRYSTAL

Cobalt Oxide (CoO)

T/K	C <sub>p</sub> <sup>a</sup>	S <sup>b</sup> - [C <sup>b</sup> - H <sup>b</sup> (T)]/T	H <sup>b</sup> - H <sup>b</sup> (T)	Standard State Pressure = p <sup>c</sup> = 0.1 MPa kJ·mol <sup>-1</sup>	log K <sub>r</sub>
0	0	INFINITE	-9.434	-238.056	INFINITE
100	19.038	0.109	-8.794	-239.590	120.593
200	45.376	30.904	-5.496	-239.458	58.025
298.15	55.279	52.993	0	-237.735	37.490
300	54.831	53.333	0.102	-237.706	37.233
400	52.932	68.698	5.439	-236.422	26.912
500	53.932	80.628	10.788	-235.342	20.751
600	54.312	90.497	16.201	-234.402	16.661
700	54.513	98.883	21.642	-233.625	13.751
800	54.819	106.180	27.107	-233.028	11.570
900	55.312	112.664	32.612	-232.570	9.879
1000	56.011	118.526	38.176	-232.209	8.527
1100	56.886	123.904	43.820	-232.056	7.423
1200	57.915	128.897	49.559	-232.027	6.502
1300	59.070	133.576	55.397	-232.131	5.701
1400	60.251	138.000	61.377	-232.348	5.050
1500	61.672	142.208	67.476	-232.671	4.467
1600	63.086	146.233	73.713	-233.707	3.958
1700	64.559	150.102	80.095	-232.966	3.510
1800	66.078	153.835	86.627	-248.354	3.105
1900	67.639	157.449	93.312	-247.588	2.726
2000	69.233	160.959	100.156	-246.676	2.386
2100	70.856	164.376	107.160	-245.615	2.080
2200	72.505	167.710	114.328	-244.401	1.803
2300	74.174	170.970	121.662	-243.033	1.551
2400	75.860	174.162	129.164	-241.508	1.322
2500	77.563	177.294	136.834	-239.825	1.112
2600	79.283	180.369	144.676	-237.981	0.920
2700	81.011	183.394	152.691	-236.459	0.744
2800	82.747	186.371	160.879	-235.306	0.582
2900	84.496	189.305	169.241	-234.473	0.432
3000	86.253	192.199	177.778	-228.974	0.294

S<sup>a</sup>(298.15 K) = 52.993 ± 0.34 J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>fus</sub> = 2103 ± 10 K  
 Δ<sub>sub</sub>H<sup>b</sup>(0 K) = -238.1 ± 0.4 kJ·mol<sup>-1</sup>  
 Δ<sub>sub</sub>H<sup>b</sup>(298.15 K) = -237.7 ± 0.4 kJ·mol<sup>-1</sup>  
 Δ<sub>sub</sub>H<sup>b</sup> = Unknown

Enthalpy of Formation

Boyle *et al.*<sup>1</sup> measured the enthalpy of combustion of metallic cobalt at 303.16 K. Their analyses of the combustion products indicated that some overoxidation of the metal had occurred. Correction of their results to correspond to CoO was made on the assumption that the excess oxygen was combined as Co<sub>3</sub>O<sub>4</sub>. Also the analyses indicated that the combustion products had attacked the silica-glass capsules, used to hold the metal samples, resulting in appreciable amounts of silicate formation. Corrections for these two side reactions amounted to three percent of the total measured energy of combustion. From these data, we derive Δ<sub>sub</sub>H<sup>b</sup>(CoO, cr, 298.15 K) = -57.0 ± 0.3 kcal·mol<sup>-1</sup>. Roth and Havokoss<sup>2</sup> also investigated calorimetrically the combustion of metallic cobalt and reported Δ<sub>sub</sub>H<sup>b</sup>(CoO, cr, 298.15 K) = -57.2 ± 0.2 kcal·mol<sup>-1</sup>.

2nd and 3rd law analyses of several equilibrium studies,<sup>3-12</sup> emf measurements,<sup>13</sup> and mass-spectrometric studies<sup>14</sup> involving CoO(cr) are discussed in the JANAF Thermochemical Tables.<sup>14</sup> Δ<sub>sub</sub>H<sup>b</sup>(CoO, cr, 298.15 K) = -56.82 ± 0.10 kcal·mol<sup>-1</sup> (-237.735 ± 0.4 kJ·mol<sup>-1</sup>) was adopted. A recent critical evaluation by Cyr *et al.*<sup>15</sup> recommended Δ<sub>sub</sub>H<sup>b</sup>(CoO, cr, 298.15 K) = -237.5 ± 0.4 kJ·mol<sup>-1</sup>, based on 2nd and 3rd law analyses. Since this value differs from the value previously adopted by JANAF by only 0.2 kJ·mol<sup>-1</sup>, and includes ten new references in the evaluation, it is adopted for the current table.

Heat Capacity and Entropy

The adopted heat capacities for CoO(cr) in the temperature range 51–298 K are those of King<sup>15</sup>. These data have a pronounced maximum at 287.3 K, at which point the heat capacity is greater than 17.6 cal·K<sup>-1</sup>·mol<sup>-1</sup>. Assayag and Bizette<sup>16</sup> also measured heat capacities for CoO(cr) between 180–400 K and reported a maximum at 298.7 K. Presumably this anomaly is of the magnetic type. Heat capacity data above 300 K are calculated from the high temperature (400–1800 K) enthalpy data of King and Christensen.<sup>15</sup> Both sets of data were smoothed by computer and joined at 298.15 K.

The value of S<sup>a</sup>(298.15 K) is obtained from the low temperature heat capacity data of King<sup>15</sup> and is based on S<sup>a</sup>(51 K) = 0.42 cal·K<sup>-1</sup>·mol<sup>-1</sup>.

Fusion Data

The adopted T<sub>fus</sub> of 2103 ± 10 K was recommended by IUPAC [20] based on the work of Coutures.<sup>21</sup>

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PREVIOUS:

CURRENT: December 1970

Cobalt Oxide (CoO)

Co<sub>3</sub>O<sub>4</sub>(cr)

Co<sub>3</sub>O<sub>4</sub>S<sub>1</sub>(cr)Cobalt Sulfate (CoSO<sub>4</sub>)M<sub>r</sub> = 154.9908

CRYSTAL (α-β)

Cobalt Sulfate (CoSO<sub>4</sub>)

S<sup>o</sup>(298.15 K) = 117.377 ± 4.2 J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>m</sub> (α → β) = 964 ± 5 K

### Enthalpy of Formation

Adami and King<sup>1</sup> determined calorimetrically the enthalpies of solution of crystalline CoO and α-CoSO<sub>4</sub> in hydrochloric acid solution. From these measurements they derived the enthalpy for the reaction CoO(cr) + H<sub>2</sub>SO<sub>4</sub>·7.068 H<sub>2</sub>O(l) → CoSO<sub>4</sub>(cr) + 8.068 H<sub>2</sub>O(l) as ΔH<sup>o</sup>(298.15 K) = -14.280 ± 0.110 kcal·mol<sup>-1</sup>. Combining this result with enthalpies of formation for CoO<sup>2</sup>, H<sub>2</sub>SO<sub>4</sub>·7.068 H<sub>2</sub>O, and H<sub>2</sub>O<sup>3</sup>, we derive ΔH<sup>o</sup>(α-CoSO<sub>4</sub>, cr, 298.15 K) = -212.3 ± 0.3 kcal·mol<sup>-1</sup> (-888.263 ± 1.3 kJ·mol<sup>-1</sup>) which is adopted.

The total pressures of SO<sub>2</sub>(g), SO<sub>3</sub>(g), and O<sub>2</sub>(g) over CoSO<sub>4</sub>(cr) in the temperature range 1100–1300 K have been determined by manometric<sup>4,5</sup> and transpiration<sup>6</sup> methods. Previous investigators<sup>4,5</sup> analyzed these data solely in terms of two equilibria, namely (A) CoSO<sub>4</sub>(cr) = CoO(cr) + SO<sub>2</sub>(g) and (B) SO<sub>3</sub>(g) = SO<sub>2</sub>(g) + 0.5 O<sub>2</sub>(g). However, Warner<sup>10</sup> has shown that CoSO<sub>4</sub> takes part in three successive, univariant, decomposition equilibria as the temperature is increased. Co<sub>2</sub>O<sub>3</sub> is the decomposition product at low temperatures (<1150 K), a mixture of Co<sub>2</sub>O<sub>3</sub> and CoO at intermediate temperatures, and CoO at high temperatures. Second and third law analyses of those points involving only equilibria (A) and (B) are given below. The appearance of Co<sub>2</sub>O<sub>3</sub> as a decomposition product was determined by comparing the oxygen partial pressures that were calculated from the total pressure data with those for the decomposition reaction (C) Co<sub>2</sub>O<sub>3</sub>(cr) → 3 CoO(cr) + 0.5 O<sub>2</sub>(g).<sup>7</sup> Espelund and Flengas<sup>8</sup> measured the Gibbs energy of reaction (A) in a high temperature solid electrolyte cell. Here, no Co<sub>2</sub>O<sub>3</sub> was formed over the entire temperature range (827–1133 K), since the oxygen pressures in the cell were too low to oxidize the CoO. Results of an analysis of these data are also given below.

Source	Reaction	Method	Data Points	T/K	ΔH <sup>o</sup> (298.15 K), kcal·mol <sup>-1</sup>	Drift	ΔH <sup>o</sup> (298.15 K), kcal·mol <sup>-1</sup>
Marchal <sup>4</sup>	A	Manometric	17	1143–1303	54.5	60.4 ± 0.5	-211.8 ± 0.8
Schenck and Raub <sup>5</sup>	A	Manometric	14	1099–1243	68.5	60.9 ± 0.7	-212.3 ± 1.0
Warner <sup>6</sup>	A	Manometric	2	1164–1175	56.9	59.3 ± 0.3	-210.8 ± 0.3
Ingraham <sup>7</sup>	A	Manometric	9	1144–1210	59.1	59.1 ± 0.1	0.04 ± 0.91
Alcock <i>et al.</i> <sup>8</sup>	D**	Transpiration	8	1131–1217	-191.1	-166.8 ± 1.4	-211.2 ± 1.5
Espelund and Flengas <sup>9</sup>	A, enf	A, enf	28	827–1177	59.5	59.5 ± 0.3	-211.0 ± 0.6

\*\* Reaction: (D) 2 CoO(cr) + 2 SO<sub>2</sub>(g) + O<sub>2</sub>(g) = 2 CoSO<sub>4</sub>(cr)

These results indicate that the Gibbs energy functions and equilibrium data are consistent within experimental error.

### Heat Capacity and Entropy

The low temperature (52–298 K) heat capacities are those reported by Weller.<sup>11</sup> No anomalies appear in these data. Heat capacities in the temperature range 300–2000 K are estimated by comparison with those for CuSO<sub>4</sub>.<sup>2</sup> S<sup>o</sup>(298.15 K) is determined from the C<sub>p</sub> data based on S<sup>o</sup>(51 K) = 1.56 + 2.75 cal·K<sup>-1</sup>·mol<sup>-1</sup>. The 1.56 is a lattice contribution, while the 2.75 is the entropy associated with the ordering of the Co<sup>2+</sup> spin moments. In assigning the magnetic entropy, it is assumed that all of the contribution remains to be extracted below the minimum temperature (52 K) of the heat capacity measurements.<sup>11</sup>

### Transition Data

The temperature (T<sub>m</sub>) and the heat (Δ<sub>tr</sub>H<sup>o</sup>) of the α-β transition for CoSO<sub>4</sub> are from the differential thermal analysis studies of Ingraham and Marier.<sup>12</sup> Other temperatures reported for the transition are 890<sup>6</sup> and 903 K.<sup>13</sup>

### Decomposition Data

T<sub>de</sub> is the temperature at which the Gibbs energy change for the process CoSO<sub>4</sub>(cr) → CoO(cr) + SO<sub>2</sub>(g) is zero.

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T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ))/T <sub>r</sub>	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )/T	Δ <sub>r</sub> H <sup>o</sup>	
0	0	0	INFINITE	-878.952	INFINITE
100	44.454	37.748	192.584	-851.311	444.679
200	80.281	80.789	126.133	-817.096	213.403
298.15	103.219	117.377	117.377	-888.263	137.075
300	103.638	118.017	117.379	-888.269	136.115
400	119.286	150.056	121.642	-890.202	97.490
500	131.545	178.049	130.182	-890.418	74.187
600	140.666	202.877	140.269	-889.584	58.689
700	152.047	225.081	151.380	-888.064	47.634
800	165.979	243.074	161.827	-886.571	39.355
900	181.534	263.190	171.702	-885.599	32.867
964.000	196.792	273.916	178.135	-885.599	32.867
964.000	157.221	216.129	178.135	ALPHA → BETA TRANSITION	
1000	158.113	281.910	181.767	-932.148	27.439
1100	160.415	297.089	191.571	-928.946	23.020
1200	162.465	311.137	200.956	-925.920	19.350
1300	164.306	324.215	209.941	-923.232	16.254
1400	165.979	336.453	218.545	-921.070	13.608
1500	167.569	347.959	226.793	-917.705	11.321
1600	169.075	358.822	234.708	-914.048	9.327
1700	170.498	369.115	242.314	-910.211	7.575
1800	171.921	378.901	249.633	-907.259	6.016
1900	173.259	388.232	256.684	-904.189	4.610
2000	174.598	397.153	263.486	-901.502	3.350

PREVIOUS:

CURRENT: December 1971

Cobalt Sulfate (CoSO<sub>4</sub>)Co<sub>3</sub>O<sub>4</sub>S<sub>1</sub>(cr)

Co<sub>3</sub>O<sub>4</sub>(cr)

M<sub>r</sub> = 240.7972 Cobalt Oxide (Co<sub>3</sub>O<sub>4</sub>)

CRYSTAL

Cobalt Oxide (Co<sub>3</sub>O<sub>4</sub>)

S°(298.15 K) = 114.29 ± 4.2 J·K<sup>-1</sup>·mol<sup>-1</sup> Δ<sub>f</sub>H°(0 K) = -896.3 ± 4.0 kJ·mol<sup>-1</sup> Δ<sub>f</sub>H°(298.15 K) = -910.0 ± 4.0 kJ·mol<sup>-1</sup>

Enthalpy of Formation

Bugden and Pratt<sup>1</sup> measured Gibbs energies of reaction for (a) 2Cu(cr) + Co<sub>3</sub>O<sub>4</sub>(cr) → 3CoO(cr) + Cu<sub>2</sub>O(cr) and (b) Ni(cr) + Co<sub>3</sub>O<sub>4</sub>(cr) → 3CoO(cr) + NiO(cr) from high temperature solid electrolytic cells. These data were subjected to 2nd and 3rd law analyses with results summarized in the following table:

Source	Reaction	Method	T/K	Δ <sub>f</sub> H°(298.15 K) kcal·mol <sup>-1</sup>			Drift	Δ <sub>f</sub> H°(298.15 K)*
				2nd law	3rd law	3rd law		
Bugden and Pratt <sup>1</sup>	a	emf	900-1150	5.1	6.3 ± 0.2	1.1	-217.5 ± 0.8	
	b	emf	850-1100	-12.0	-10.6 ± 0.2	1.3	-217.1 ± 0.8	
Footo and Smith <sup>3</sup>	c	Manometric	1073-1243	34.5	47.2 ± 1.4	10.6 ± 1.3	-217.7 ± 1.5	
Watanabe <sup>4</sup>	c	Manometric	1128-1233	38.1	47.9 ± 0.7	8.3 ± 0.8	-218.4 ± 1.0	
Chufarov <i>et al.</i> <sup>5</sup>	c	Manometric	973-1173	27.9	46.4 ± 2.9	17.0 ± 0.6	-216.9 ± 3.0	
Balakirev and Chufarov <sup>6</sup>	c	Manometric	923-1173	33.8	46.1 ± 2.5	11.3 ± 2.5	-216.6 ± 3.0	
Rother and Paladine <sup>7</sup>	c	Manometric	1139-1220	36.4	47.1 ± 0.6	9.0 ± 2.0	-217.6 ± 1.0	
Ingraham <sup>8</sup> Set I	c	Manometric	1101-1159	41.4	46.8 ± 0.2	4.5 ± 0.4	-217.3 ± 0.5	
	c	Manometric	1086-1219	35.6	46.9 ± 0.8	9.7 ± 0.2	-217.4 ± 1.0	
O'Bryan and Parravano <sup>9</sup>	c	X-ray & Wt. Loss	1073-1243	40.3	47.3 ± 0.8	5.9	-217.8 ± 1.0	

\*3rd law values based on Δ<sub>f</sub>H°(CoO,cr, 298.15 K) = -56.82 ± 0.1 kcal·mol<sup>-1</sup>.

Both sets of emf data are much more compatible with the adopted functions than the dissociation pressure data (refer to the discussion below). The results obtained with the Cu/Cu<sub>2</sub>O reference couple are judged to be more reliable and lead to the adopted enthalpy of formation, Δ<sub>f</sub>H°(Co<sub>3</sub>O<sub>4</sub>,cr, 298.15 K) = -217.5 ± 1.0 kcal·mol<sup>-1</sup>, when used in conjunction with JANAF<sup>2</sup> enthalpies of formation for CoO and Cu<sub>2</sub>O.

Equilibrium oxygen pressures for the reaction (c) Co<sub>3</sub>O<sub>4</sub>(cr) + 0.5 O<sub>2</sub>(g) = 3CoO(cr) have been determined by numerous investigators.<sup>3-9</sup> 2nd and 3rd law analyses of these data are given in the above table. Within each set the 2nd and 3rd law Δ<sub>f</sub>H°(298.15 K) values are not in agreement, and all sets contain large positive drifts. Warner<sup>10</sup> has suggested that these discrepancies arise as a result of an error in the measured standard entropy<sup>11</sup> for Co<sub>3</sub>O<sub>4</sub>. However, once the magnetic contribution is included (see entropy write-up) the real error in this value is probably no greater than one cal·K<sup>-1</sup>·mol<sup>-1</sup>. The other possible source of error is lack of true equilibrium conditions. Recent thermogravimetric, X-ray, and kinetic,<sup>12</sup> studies of the Co<sub>3</sub>O<sub>4</sub>-CoO-O<sub>2</sub> system all point to an irreversible reaction. Therefore, no weight has been given to the dissociation pressure data in our evaluation.

Heat Capacity and Entropy

The low temperature heat capacities (54-296.3 K) are those reported by King.<sup>11</sup> Heat capacities in the temperature range 300-1000 K are calculated from the high temperature enthalpy data of King and Christensen,<sup>13</sup> a constrained curve fitting technique was used to join smoothly these data with the low temperature data at 298 K. No anomalies appear in either set of data. Roth<sup>14</sup> observed a maximum in the magnetic susceptibility of Co<sub>3</sub>O<sub>4</sub> at 40 K, while Mossbauer studies by Kundig *et al.*<sup>15</sup> indicated a Neel temperature of 33.0 ± 1.0 K. With the assumption that Co<sub>3</sub>O<sub>4</sub> is a normal 2-3 spinel,<sup>16</sup> this transition can be associated with the antiferromagnetic ordering of the Co<sup>2+</sup> ion spin moments. Therefore, the entropy is based on S°(51 K) = 1.36 + 2.75 = 4.11 cal·K<sup>-1</sup>·mol<sup>-1</sup>, where 1.36 is a lattice contribution and 2.75 is the magnetic entropy. In assigning the magnetic entropy, it is assumed that all of the contribution remains to be extracted below the minimum temperature (54 K) of the heat capacity measurements.

Decomposition Data

T<sub>dec</sub> is the temperature at which the Gibbs energy change for the process Co<sub>3</sub>O<sub>4</sub>(cr) → 3CoO(cr) + 0.5 O<sub>2</sub>(g) is zero.

References

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T/K	Enthalpy Reference		Temperature = T, = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup>	-(G°-H°(T))/T	H°-H°(T)	Δ <sub>f</sub> H°	Δ <sub>f</sub> G°	
0	0	0	INFINITE	-17.968	-896.309	-896.309	INFINITE
100	34.368	31.487	198.112	-16.663	-902.377	-868.560	53.589
200	87.595	72.039	124.547	-10.501	-907.767	-852.928	217.468
298.15	123.051	114.286	114.286	0	-910.070	-852.928	139.258
300	123.512	115.049	114.286	0.228	-910.038	-852.928	138.275
400	142.666	153.637	119.423	13.694	-910.220	-755.468	98.654
500	152.850	186.590	129.647	28.471	-909.774	-716.825	74.886
600	162.808	215.325	141.580	44.247	-908.999	-678.902	59.051
700	173.628	241.224	153.992	61.062	-907.902	-649.041	47.753
800	185.272	265.161	166.410	79.001	-906.531	-624.601	39.280
900	197.552	287.688	178.645	98.159	-905.043	-603.706	32.706
1000	210.296	309.158	190.650	118.528	-902.293	-585.712	27.460
1100	223.384	329.814	202.350	140.210	-899.139	-569.203	23.183
1200	236.727	349.821	213.809	163.214	-895.639	-550.998	19.631
1300	250.262	369.303	225.024	187.562	-892.206	-540.087	16.638
1400	263.943	388.349	236.012	213.272	-889.197	-537.422	14.082
1500	277.742	407.029	246.793	240.355	-881.838	-541.108	11.878

PREVIOUS: December 1970

CURRENT: December 1971

Cobalt Oxide (Co<sub>3</sub>O<sub>4</sub>)

Co<sub>3</sub>O<sub>4</sub>(cr)