Iron Oxide, Wüstite (Fe0.947O)   CRYSTAL M_r = 68.8865   Iron Oxide, Wüstite (Fe0.947O)   Fe0.947O1(cr)

$S°(298.15\ K) = 57.588 \pm 0.42\ \text{J·K}^{-1}\text{·mol}^{-1}$
$T_{fus} = 1650\ K$

$\Delta_f H°(0\ K) = -267.123 \pm 0.84\ \text{kJ·mol}^{-1}$
$\Delta_f H°(298.15\ K) = -266.270 \pm 0.84\ \text{kJ·mol}^{-1}$
$\Delta_{fus} H° = 31.338\ \text{kJ·mol}^{-1}$

Standard State Pressure = $p°$ = 0.1 MPa

Enthalpy Reference Temperature = T_r = 298.15 K

T/K	$C°_p$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹·mol⁻¹				kJ·mol⁻¹		
0	0.	0.	INFINITE	-9.462	-267.123	-267.123	INFINITE
100	23.336	12.294	98.526	-8.623	-268.136	-260.126	135.876
187.670	58.206	35.752	63.498	-5.207	C, LAMBDA MAXIMUM		
187.670	58.196	35.754	63.498	-5.207	TRANSITION		
200	45.966	38.989	61.893	-4.581	-267.224	-252.274	65.887
298.15	48.116	57.588	57.588	0.	-266.270	-245.143	42.948
300	48.183	57.886	57.589	0.089	-266.252	-245.012	42.660
400	50.380	72.065	59.507	5.023	-265.292	-238.078	31.090
500	51.848	83.470	63.196	10.137	-264.409	-231.379	24.172
600	53.028	93.030	67.393	15.382	-263.666	-224.845	19.575
700	54.070	101.283	71.658	20.737	-263.088	-218.423	16.299
800	55.041	108.567	75.825	26.193	-262.723	-212.071	13.847
900	55.969	115.104	79.833	31.744	-262.690	-205.745	11.941
1000	56.873	121.048	83.661	37.386	-263.275	-199.395	10.415
1100	57.760	126.510	87.312	43.118	-264.641	-192.927	9.161
1200	58.630	131.573	90.792	48.938	-265.416	-186.391	8.113
1300	59.496	136.300	94.112	54.844	-264.562	-179.840	7.226
1400	60.358	140.741	97.286	60.837	-263.716	-173.355	6.468
1500	61.212	144.934	100.324	66.915	-262.878	-166.930	5.813
1600	62.065	148.912	103.238	73.079	-262.046	-160.561	5.242
1700	62.787	152.699	106.037	79.325	-262.124	-154.225	4.739
1800	63.304	156.303	108.730	85.631	-261.650	-147.892	4.292
1900	63.696	159.736	111.325	91.982	-274.573	-140.919	3.874
2000	64.015	163.012	113.828	98.368	-274.427	-133.889	3.497
2100	64.238	166.141	116.245	104.781	-274.265	-126.866	3.156
2200	64.434	169.134	118.582	111.214	-274.094	-119.850	2.846
2300	64.601	172.002	120.842	117.666	-273.916	-112.844	2.563
2400	64.740	174.754	123.032	124.134	-273.733	-105.844	2.304
2500	64.852	177.399	125.154	130.614	-273.549	-98.853	2.065

Enthalpy of Formation

The chemical equilibria in the Fe-C-O and Fe-H-O system have been studied by many investigators. Using the reported equilibrium constants for the following two reactions (A) $Fe_{0.947}O(cr) + CO(g) = 0.947Fe(cr) + CO_2(g)$ and (B) $Fe_{0.947}O(cr, 1) + H_2(g) = 0.947Fe(cr) + H_2O(g)$, the corresponding enthalpy changes $\Delta_f H°$ were evaluated by both the 2nd and 3rd law methods. Based on the 3rd law values for $\Delta_f H°$, the $\Delta_f H°$(Wustite, cr, 298.15 K) values were also calculated. The results obtained are presented as follows.

Source	Reaction	T/K	$\Delta_f H°$(298.15 K), kcal·mol⁻¹ 2nd law	3rd law	$\Delta_f H°$(298.15 K) kcal·mol⁻¹
Eastman[1]	A	873.2-1273.2	-3.80 ± 0.01	-4.01	-63.63
Eastman–Evans[2]	A	973.2-1273.2	-4.02 ± 0.01	-4.03	-63.61
Eastman[1]	B	873.2-1273.2	6.50 ± 0.12	5.90	-63.70
Eastman–Evans[2]	B	973.2-1273.2	5.81 ± 0.01	5.07	-62.86
Emmett–Schultz[3]	B	873.2-1273.2	5.95 ± 0.07	5.82	-63.62
Britzke et al.[4]	B	1123.2-1498.2	-2.25 ± 0.03	4.26	-62.06
Jominy–Murphy[5]	B	1360.0-1646.0	5.01 ± 0.61	6.01	-63.81
Chipman–Marshall[6]	B	1438.2-1633.2	5.03 ± 0.34	5.85	-62.83
Chipman–Marshall[6]	B	1653.2-1787.2	-2.61 ± 0.77	-0.02	-61.87
Jominy–Murphy[5]	B	1698.0-1700.0		-0.87	-62.72
Britzke et al.[4]	C	1123.0 1473.0	-129.08 ± 0.18	-126.28	-63 14

Britzke et al.[4] also determined the equilibrium pressures for the reaction (C) $1.894\ Fe(cr) + O_2(g) = 2Fe_{0.947}O(cr)$. The corresponding $\Delta_f H°$(298.15 K) for Wustite was evaluated based on the 3rd law value for $\Delta_f H°$(298.15 K). The adopted value of $\Delta_f H°$(Wustite, cr, 298 15 K) is the weighted average of the $\Delta_f H°$(298 15 K) listed in the above table.

Heat Capacity and Entropy

The low temperature (54.37-298.16 K) heat capacities were measured by Todd and Bonnickson.[7] The high temperature (298-1650 K) heat capacities were determined by Coughlin et al.[8] The two sets of $C°_p$ data were plotted and joined smoothly at 298.15 K. The $C°_p$ values above 1650 K were obtained by graphical extrapolation. The low temperature (70.7-279.8 K) $C°_p$'s were also reported by Millar.[9] $S°$(298.15 K) was derived from the low-temperature heat capacities, based on $S°$(52 K) = 0.696 cal·K⁻¹·mol⁻¹. Todd and Bonnickson[7] added 0.41 cal·K⁻¹·mol⁻¹, the amount calculated for completely random distribution of the vacant Fe spaces in the Wustite lattice. However, the Gibbs energy functions derived from $S°$(52 K) = 0.696 cal·K⁻¹·mol⁻¹ give better agreement between 2nd and 3rd law values for $\Delta_f H°$ than those derived from $S°$(52 K) = 1.11 cal·K⁻¹·mol⁻¹. Therefore, the value 0.41 cal·K⁻¹·mol⁻¹ was not added here.

Fusion Data

T_{fus} and $\Delta_{fus} H°$ were taken from Coughlin et al.[8] T_{fus} was reported as 1372°C (1645 K) by Darken and Gurry[9] and as 1369°C (1642 K) by Chipman and Marshall.[6]

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CURRENT June 1965

PREVIOUS:

Iron Oxide, Wüstite (Fe0.947O)   Fe0.947O1(cr)

Iron Sulfide, Pyrrhotite (Fe0.877S)   CRYSTAL $M_r = 81.038$

$S°(298.15\ K) = 60.799 \pm 0.4\ J\cdot K^{-1}\cdot mol^{-1}$
$T_{m2} = 598 \pm 3\ K$

$\Delta_f H°(0\ K) = -106.31 \pm 1.7\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -105.44 \pm 1.7\ kJ\cdot mol^{-1}$
$\Delta_{trs} H° = 0.398 \pm 0.84\ kJ\cdot mol^{-1}$

Enthalpy of Formation

The adopted value of $\Delta_f H°(298.15\ K)$ is based on the calorimetric determination of Stolyarova and Bezmen[1] assuming that their reported value refers to 298.15 K. This value came from an average of eight determinations of $\Delta_f H°$ for $Fe_{0.877}S(cr) + Zn(cr) \rightarrow ZnS(cr) + 0.877\ Fe(cr)$.

In the composition range $y = 0.095$ to 0.145, Bugli et al.[2] determined $\Delta_f H°(433\ K) = -14.4\Delta y\ (0.025)$ kcal·mol^{-1} for $Fe_{0.877}S(cr)$. Using $y = x/(1-x)$ we calculate that $\Delta_f H°(433\ K) = -14.76x + 0.36$ kcal·mol^{-1} for $(1-x)FeS(cr) + xS(l) \rightarrow Fe_{1-x}S(cr)$ in this same composition range. Using $x = 0.123$ and auxiliary JANAF data[3] we can then calculate $\Delta_f H°(Fe_{0.877}S, cr) = -22.1$ kcal·mol^{-1} based on Bugli's data. The difference between this value of $\Delta_f H°(298.15\ K)$ and that of Stolyarova and Bezmen is probably due to different morphology of the products; Bugli et al. state they are uncertain as to the exact nature of their product. Due to the complicated and kinetically slow phase behavior of $Fe_{0.877}S$, it appears they may not have obtained the pure monoclinic product.

Heat Capacity and Entropy

The adopted heat capacities from 6–350 K are based on our analysis of the $C°_p$ data of Gronvold et al.[4] Two small anomalies in the $C°_p$ curve, for which there is no obvious explanation, were observed near 8 and 30 K.[4] These lead to entropy increments of 0.003 and 0.03 cal·K^{-1}·mol^{-1}, respectively. Since there are no measured $C°_p$ or enthalpy data above 350 K, the $C°_p$ is estimated via the following procedure. Above TB, $C°_p$ is estimated as $C°_p(Fe_{0.877}S, cr) = C°_p(FeS, cr) - 0.123\ C°_p(Fe, cr)$ using auxiliary JANAF data.[3] Since the $T\alpha$ transition present in FeS(cr, troilite) is not present in pyrrhotite of composition $Fe_{0.877}S$[3] the heat capacity is assumed to be linear between 350 and 598 K where $C°_p(598\ K)$ is estimated via the procedure outlined above. Hirone et al.[5] observed non-linear behavior for $C°_p$ of $Fe_{0.90}S$ from 513 to 593 K.

The value of $S°(298.15\ K)$ is derived from the appropriate integration of $C°_p$ data assuming $S°(6\ K) = 0.0007$ cal·K^{-1}·mol^{-1}.

Phase Data

The mineral pyrrhotite has a composition range extending from FeS to $Fe_{0.877}S$ (~Fe_7S_8), the name troilite is reserved for the stoichiometric FeS composition. The data presented in this table refer to the iron poor composition limit which is found to be $Fe_{0.877}S$ below T_{m2}.[6] For stoichiometric FeS there are 3 crystalline polymorphs designated α, β, γ from low to high temperature, where the α β transition is designated T_{m1} and the β-γ transition is designated T_{m2}. We retain this nomenclature for $Fe_{0.877}S$ while recognizing that the α phase does not exist for this composition. Hirone et al.[5] found TB and ΔHB° to be independent of composition so we adopt the same values as for FeS(cr, troilite).[3] The transition at 411 K (T_{m1}) in FeS was found to be non-existent i compositions containing less iron than $Fe_{0.9}S$[3] so it will not be present in $Fe_{0.877}S$. The crystal structure of $Fe_{0.877}S$ is hexagonal above T_{m2} while the stable form below T_{m2} is monoclinic.[6] The conversion from hexagonal to monoclinic when cooling through T_{m2} is kinetically slow and even annealing for several months may not be sufficient for complete conversion.[6,7]

References

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[7]H. Nakazawa and N. Morimoto, Mat. Res. Bull. 6, 345 (1971).

Iron Sulfide, Pyrrhotite (Fe0.877S)

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

T/K	$C°_p$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	-9.241	-106.313	-106.313	INFINITE
100	25.899	18.565	99.374	-8.081	-106.214	-106.286	55.518
200	42.257	42.394	65.139	-4.549	-105.875	-106.478	27.809
298.15	49.883	60.799	60.799	0.	-105.437	-106.863	18.722
300	50.000	61.108	60.800	0.092	-105.427	-106.872	18.608
400	56.149	76.334	62.835	5.399	-107.022	-107.353	14.019
500	62.383	89.531	66.880	11.325	-107.526	-107.381	11.218
598.000	68.563	101.232	71.565	17.741			
598.000	58.175	101.897	71.565	18.139	BETA<-->GAMMA TRANSITION		
600	58.116	102.091	71.666	18.255	-106.887	-107.365	9.347
700	55.564	110.847	76.659	23.932	-107.474	-107.403	8.015
800	53.848	118.146	81.401	29.396	-108.391	-107.335	7.008
900	52.886	124.432	85.841	34.732	-162.845	-106.047	6.155
1000	52.007	129.922	89.980	39.941	-163.655	-99.702	5.208
1100	55.396	135.035	93.845	45.309	-165.108	-93.221	4.427
1200	59.120	140.016	97.486	51.036	-165.731	-86.673	3.773
1300	62.676	144.882	100.945	57.118	-164.572	-80.130	3.220
1400	67.195	149.686	104.255	63.603	-163.098	-73.687	2.749
1500	72.676	154.503	107.444	70.589	-161.213	-67.364	2.346
1600	79.161	159.398	110.538	78.177	-158.813	-61.182	1.997
1700	86.107	164.398	113.558	86.428	-156.671	-55.152	1.695
1800	94.517	169.551	116.525	95.447	-153.309	-49.274	1.430

Iron (Fe)

$A_r = 55.847$ Iron (Fe)

Fe₁(ref)

REFERENCE STATE

0	to	1184	K crystal, alpha
1184	to	1665	K crystal, gamma
1665	to	1809	K crystal, delta
1809	to	3133.345	K liquid
above		3133.345	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⁻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	-4.507	0.	0.	0.
100	12.101	6.065	46.905	-4.084	0.	0.	0.
200	21.588	17.949	29.524	-2.315	0.	0.	0.
298.15	25.094	27.321	27.321	0.	0.	0.	0
300	25.140	27.476	27.321	0.046	0.	0.	0.
400	27.386	35.021	28.335	2.674	0.	0.	0.
500	29.702	41.377	30.323	5.527	0.	0.	0.
600	32.049	46.997	32.642	8.613	0.	0.	0.
700	34.602	52.119	35.063	11.939	0.	0.	0.
800	37.949	56.940	37.498	15.553	0.	0.	0.
900	43.095	61.679	39.922	19.582	0.	0.	0.
1000	54.434	66.672	42.342	24.329	0.	0.	0.
1042.000	83.680	69.245	43.372	26.960	C_p LAMBDA MAXIMUM TRANSITION		
1042.000	83.681	69.245	43.372	26.960			
1100	46.401	72.062	44.815	29.972	0.	0.	0.
1184.000	41.422	75.260	46.865	33.619	ALPHA <--> GAMMA TRANSITION		0.
1184.000	33.882	76.020	46.865	34.519			
1200	34.016	76.476	47.257	35.062	0.	0.	0.
1300	34.853	79.231	49.612	38.505	0.	0.	0.
1400	35.690	81.845	51.822	42.033	0.	0.	0.
1500	36.526	84.336	53.907	45.643	0.	0.	0.
1600	37.363	86.720	55.884	49.338	0.	0.	0.
1665.000	37.907	88.218	57.117	51.784	GAMMA <--> DELTA TRANSITION		
1665.000	41.112	88.721	57.117	52.621			
1700	41.463	89.580	57.776	54.066	0.	0.	0.
1800	42.468	91.978	59.610	58.263	0.	0.	0.
1809.000	42.558	92.190	59.772	58.645	DELTA <--> LIQUID TRANSITION		
1809.000	46.024	99.823	59.772	72.452			
1900	46.024	102.082	61.744	76.641	0.	0.	0.
2000	46.024	104.442	63.821	81.243	0.	0.	0.
2100	46.024	106.688	65.809	85.845	0.	0.	0.
2200	46.024	108.829	67.716	90.448	0.	0.	0.
2300	46.024	110.875	69.549	95.050	0.	0.	0.
2400	46.024	112.833	71.312	99.653	0.	0.	0.
2500	46.024	114.712	73.010	104.255	0.	0.	0.
2600	46.024	116.517	74.649	108.857	0.	0.	0.
2700	46.024	118.254	76.232	113.460	0.	0.	0.
2800	46.024	119.928	77.763	118.062	0.	0.	0.
2900	46.024	121.543	79.245	122.665	0.	0.	0.
3000	46.024	123.103	80.681	127.267	0.	0.	0.
3133.345	46.024	125.105	82.529	133.404	LIQUID <--> IDEAL GAS		
3133.345	26.642	236.674	82.530	482.989	FUGACITY - 1 bar		
3200	26.856	237.237	85.746	484.772	0.	0.	0.
3400	27.511	238.885	94.706	490.208	0.	0.	0.
3600	28.192	240.477	102.761	495.778	0.	0.	0.
3800	28.905	242.020	110.050	501.487	0.	0.	0.
4000	29.654	243.521	116.686	507.342	0.	0.	0.
4200	30.442	244.987	122.761	513.351	0.	0.	0.
4400	31.270	246.422	128.349	519.521	0.	0.	0.
4600	32.142	247.831	133.514	525.862	0.	0.	0.
4800	33.058	249.219	138.306	532.381	0.	0.	0.
5000	34.022	250.587	142.770	539.088	0.	0.	0.
5200	35.040	251.941	146.943	545.993	0.	0.	0.
5400	36.120	253.284	150.856	553.108	0.	0.	0.
5600	37.274	254.618	154.538	560.446	0.	0.	0.
5800	38.513	255.947	158.012	568.024	0.	0.	0.
6000	39.853	257.275	161.299	575.858	0.	0.	0.

PREVIOUS: March 1978 (1 atm)

CURRENT: March 1978 (1 bar)

Fe₁(ref)

Iron (Fe)

Iron, Alpha-Delta (Fe)

CRYSTAL(α–δ)

$A_r = 55.847$ Fe (cr)

$S°(298.15\ K) = 27.32 \pm 0.13\ \mathrm{J \cdot K^{-1} \cdot mol^{-1}}$
$T_{trs1} = 1042 \pm 1\ K$ (Curie temp)
$T_{trs2} = 1184 \pm 3\ K$ (α–γ)
$T_{trs3} = 1665 \pm 3\ K$ (γ–δ)
$T_{fus} = 1809 \pm 5\ K$ (δ–l)

$\Delta_f H°(0\ K) = 0\ \mathrm{kJ \cdot mol^{-1}}$
$\Delta_f H°(298.15\ K) = 0\ \mathrm{kJ \cdot mol^{-1}}$
$\Delta_{trs1} H° = 0\ \mathrm{kJ \cdot mol^{-1}}$
$\Delta_{trs2} H° = 0.900 \pm 0.042\ \mathrm{kJ \cdot mol^{-1}}$
$\Delta_{trs3} H° = 0.837 \pm 0.084\ \mathrm{kJ \cdot mol^{-1}}$
$\Delta_{fus} H° = 13.807 \pm 0.837\ \mathrm{kJ \cdot mol^{-1}}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The current literature was surveyed by Hultgren.[1] Smoothed low temperature heat capacity values are obtained by fitting the data[2-7] graphically and with orthogonal polynomials over selected overlapping temperature intervals. Using $S°(20\ K) = 0.0364\ \mathrm{cal\ K^{-1}\ mol^{-1}}$, we integrate over the adopted smoothed heat capacity values to obtain $S°(298.15\ K) = 6.529\ \mathrm{cal\ K^{-1}\ mol^{-1}}$. An uncertainty of 0.015 cal K^{-1} mol^{-1} arises due to the choice of heat capacity values in the region 20-55 K. In this region there is considerable disagreement between the reported heat capacity values of Eucken and Werth,[2] Simon and Swain,[3] and those of Duyckaerts[4] and Keesom and Kurrelmeyer.[5] An additional uncertainty of 0.01 cal K^{-1} mol^{-1} results from the differences in the heat capacity data of Kelley[6] and Stepakoff and Kaufman.[7]

The heat capacity and enthalpy studies above room temperature are numerous. A bibliography of all known studies (including low temperature studies) is available on request. The adopted heat capacity values above 400 K are those selected by Hultgren[8] and Orr and Chipman.[9] The method of orthogonal polynomials is used to join smoothly the low and high temperature heat capacity values. The smooth heat capacity values for metastable α-Fe in the range 1184-1665 K are adjusted from those of Hultgren[8] so as to yield the proper entropy values for γ-Fe. The available heat capacity/enthalpy data show differences up to 10% in $C°_p$ for δ-Fe with the major discrepancies being different slopes in $dC°_p/dT$.

Transition Data

The enthalpies of the α-γ transition at 1184 K and the γ-δ transition at 1665 K are those selected by Hultgren[8] and Orr and Chipman.[9] The α or and δ phase has a bcc structure whereas the γ phase has a fcc structure.

Fusion Data

Refer to the liquid table for details.

Sublimation Data

The value adopted for the enthalpy of sublimation is that selected by Hultgren[8] and is based on a 2nd and 3rd law analysis of sublimation data over γ-Fe. Refer to the ideal gas table for details.

References

[1] R Hultgren, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, private communication.
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Iron, Alpha-Delta (Fe)

| | 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	-4.507	0.	0.	0.
100	12.101	6.065	46.905	-4.084	0.	0.	0.
200	21.588	17.949	29.524	-2.315	0.	0.	0.
250	23.742	23.018	27.727	-1.177	0.	0.	0.
298.15	25.094	27.321	27.321	0.	0.	0.	0.
300	25.140	27.476	27.321	0.046	0.	0.	0.
350	26.287	31.439	27.632	1.333	0.	0.	0.
400	27.386	35.021	28.335	2.674	0.	0.	0.
450	28.518	38.312	29.263	4.072	0.	0.	0.
500	29.702	41.377	30.323	5.527	0.	0.	0.
600	32.049	46.997	32.642	8.613	0.	0.	0.
700	34.602	52.119	35.063	11.939	0.	0.	0.
800	37.949	56.940	37.498	15.553	0.	0.	0.
900	43.095	61.679	39.922	19.582	0.	0.	0.
1000	54.434	66.672	42.342	24.329	0.	0.	0.
1042.000	83.680	69.245	43.372	26.960	0.	0.	0.
					C_p LAMBDA MAXIMUM TRANSITION		
1042.000	83.681	69.245	43.372	26.960	0.	0.	0.
1100	46.401	72.062	44.815	29.972	0.	0.	0.
					─ ─ ALPHA <--> GAMMA ─ ─		
1184.000	41.422	75.260	46.865	33.619			
1200	40.794	75.830	47.249	34.298	-0.764	0.010	0.001
1300	38.493	78.985	49.571	38.238	-0.267	0.052	-0.002
1400	38.535	81.830	51.775	42.077	0.044	0.065	-0.002
1500	39.455	84.518	53.869	45.974	0.330	0.056	-0.002
1600	40.459	87.097	55.866	49.969	0.631	0.029	-0.001
					─ ─ GAMMA <--> DELTA ─ ─		
1665.000	41.112	88.721	57.117	52.620			
1700	41.463	89.580	57.776	54.065	-0.001	0.	0.
1800	42.468	91.978	59.610	58.262	-0.001	0.	0.
					─ ─ DELTA <--> LIQUID ─ ─		
1809.000	42.558	92.190	59.772	58.645			
1900	43.472	94.301	61.375	62.559	-14.082	0.702	-0.019
2000	44.476	96.556	63.078	66.956	-14.287	1.486	-0.039
2100	45.480	98.751	64.725	71.454	-14.391	2.277	-0.057
2200	46.484	100.889	66.320	76.052	-14.395	3.071	-0.073

Iron, Alpha-Delta (Fe)   Fe₁(cr)

Iron, Gamma (Fe) CRYSTAL(γ) $A_r = 55.847$ Iron, Gamma (Fe) Fe₁(cr)

$S°(298.15\ K) = 35.545\ J\cdot K^{-1}\cdot mol^{-1}$
$T_{trs1} = 1184 \pm 3\ K\ (\alpha\to\gamma)$
$T_{trs2} = 1665 \pm 3\ K\ (\gamma\to\delta)$

$\Delta_f H°(298.15\ K) = 7.788\ kJ\cdot mol^{-1}$
$\Delta_{trs1}H° = 0.900 \pm 0.042\ kJ\cdot mol^{-1}$
$\Delta_{trs2}H° = 0.837 \pm 0.084\ kJ\cdot mol^{-1}$

Enthalpy of Formation

The enthalpy of formation at 298.15 K is obtained from that of Fe(α) by adding $\Delta_{trs1}H°$ and the difference between $H°(1184)-H°(298.15\ K)$ of Fe(α) and Fe(γ).

Heat Capacity and Entropy

A current literature survey by Hultgren[1] yielded approximately twenty heat capacity/enthalpy studies which gave information as to the heat capacity of γ-Fe in the stable and metastable region. A listing of these studies is available on request. We adopt the heat capacity values chosen by Hultgren[2] and Orr and Chipman.[3] These values are based primarily on the studies by Dench and Kubaschewski,[4] Braun and Kohlhaas,[5] and Wallace et al.[6] However, all the available heat capacity/enthalpy data show discrepancies up to 5% (in $C_p°$), with the major discrepancies appearing as different slopes in $C_p°$ vs T plots. Values are not extended below 298.15 K due to the lack of substantial data in this metastable region. The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

Transition Data

Refer to the Fe(α, δ) table.[7]

References

[1]R. Hultgren, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, personal communication.
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T/K	Enthalpy Reference Temperature = T_r = 298.15 K ($J\cdot K^{-1}\cdot mol^{-1}$)				Standard State Pressure = $p°$ = 0.1 MPa ($kJ\cdot mol^{-1}$)		
	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0							
100							
200							
250							
298.15	26.469	35.545	35.545	0.	7.788	5.336	-0.935
300	26.485	35.709	35.546	0.049	7.790	5.321	-0.926
350	26.903	39.823	35.870	1.384	7.839	4.905	-0.732
400	27.322	43.443	36.594	2.739	7.853	4.484	-0.586
450	27.740	46.685	37.539	4.116	7.832	4.064	-0.472
500	28.158	49.629	38.603	5.513	7.774	3.648	-0.381
600	28.995	54.837	40.885	8.371	7.546	2.842	-0.247
700	29.832	59.369	43.209	11.312	7.161	2.086	-0.156
800	30.669	63.408	45.486	14.337	6.572	1.398	-0.091
900	31.506	67.068	47.684	17.446	5.652	0.802	-0.047
1000	32.342	70.431	49.792	20.638	4.097	0.338	-0.018
1100	33.179	73.553	51.812	23.915	1.730	0.091	-0.004
1184.000	33.882	76.020	53.443	26.731	--- ALPHA <--> GAMMA ---		
1200	34.016	76.476	53.747	27.274	0.	0.	0.
1300	34.853	79.231	55.602	30.718	0.	0.	0.
1400	35.690	81.845	57.384	34.245	0.	0.	0.
1500	36.526	84.336	59.099	37.856	0.	0.	0.
1600	37.363	86.720	60.751	41.550	0.		
1665.000	37.907	88.218	61.794	43.996	--- GAMMA <--> DELTA ---		
1700	38.200	89.010	62.346	45.328	-0.950	0.019	-0.001
1800	39.037	91.217	63.889	49.190	-1.285	0.085	-0.002
1900	39.874	93.350	65.384	53.136	-15.717	0.873	-0.024
2000	40.710	95.417	66.834	57.165	-16.290	1.761	-0.046
2100	41.547	97.423	68.243	61.278	-16.780	2.676	-0.067
2200	42.384	99.375	69.614	65.474	-17.186	3.612	-0.086

Iron (Fe)   LIQUID   Fe₁(l) $A_r = 55.847$

$S°(298.15 \text{ K}) = [34.763]$ J·K⁻¹·mol⁻¹
$T_{fus} = 1809 \pm 5$ K (δ–l)

$\Delta_f H°(298.15 \text{ K}) = [12.395]$ kJ·mol⁻¹
$\Delta_{fus} H° = 13.807 \pm 0.4$ kJ·mol⁻¹

Enthalpy of Formation
The enthalpy of formation at 298.15 K is calculated from that of the combined phase crystal (α–γ–δ) by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(1809 \text{ K})–H°(298.15 \text{ K})$, between the crystal and liquid.

Heat Capacity and Entropy
The heat capacity of the liquid is taken to be 11.0 cal·K⁻¹·mol⁻¹ as in Hultgren[1] and Orr and Chipman.[2] We adopt this value in the real liquid region as well as in the extrapolated region to 1200 K and to 3500 K. Below 1200 K, heat capacity values are chosen so as to form a curve which joins smoothly the α–Fe heat capacity values in the range 298–500 K. The entropy is calculated in a manner analogous to that used for the enthalpy of formation. A current literature survey[3] revealed numerous heat capacity and enthalpy studies in the liquid region which yielded heat capacity values in the range 8.0 to 12.4 cal·K⁻¹·mol⁻¹ as given in the table below. The more recent studies by Braun et al.,[10] using a quasi-adiabatic calorimeter suggest $C°_p = 10.938$ cal·K⁻¹·mol⁻¹ whereas the levitation calorimetric enthalpy measurements of Margrave et al.[12,14] suggest 10.29 ± 0.29 and 11.138 ± 0.43 cal·K⁻¹·mol⁻¹ respectively.

Fusion Data
The adopted T_{fus} and $\Delta_{fus}H°$ values are those selected by Hultgren[1] and Orr and Chipman;[2] 1809 ± 5 K and 3300 ± 100 cal·mol⁻¹, respectively. Reported values for $\Delta_{fus}H°$ vary from a low of 2760 to a high of 3865 cal·mol⁻¹, as given in the table below.

Vaporization Data
The boiling point is calculated from the adopted thermodynamic functions and the chosen enthalpy of sublimation so that the Gibbs energy functions calculated by integration of the crystal–liquid data and by statistical methods for the gas phase are equal at T_{vap}.

Reference	Year	Calorimetric Method	T_{fus}, K	$\Delta_{fus}H°$ kcal·mol⁻¹	$C°_p(l)$ cal·K⁻¹·mol⁻¹	T/K
4	1918	drop	1801	2760		373 – 1873
5	1926, 1929	mixture	1800	3865	11.96	373 – 1906
6	1927	drop	1801	3595	12.398	370 – 1860
7	1956	mixture	1806	3658	11.2	1273 – 1923
8	1962	drop	1809 ± 1	3292 ± 80	8.0	1665 – 2210
9	1966	drop	1808	3298 ± 100	11.226	1720 – 1875
10	1965 – 1968	quasi adiab.	1809	3442 ± 50	9.766	300 – 1900
11	1971	exploding wire		3256	10.038	
12	1971	levitation		3307 ± 70	10.29 ± 0.29	1804 – 2142
13	1974	pulse	1808 ± 5			
14	1975	levitation	1811	3370 ± 90	11.138 ± 0.43	

References
[1] R. Hultgren et al., "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals, Metals Park, Ohio, (1973).
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Iron (Fe)   Fe₁(l)

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

T/K	$C°_p$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
0	0	0					
100							
200							
250							
298.15	25.096	34.763	34.763	0.	12.395	10.177	-1.783
300	25.142	34.918	34.764	0.046	12.395	10.163	-1.769
350	26.254	38.877	35.074	1.331	12.394	9.791	-1.461
400	27.384	42.457	35.776	2.672	12.393	9.419	-1.230
450	28.542	45.749	36.704	4.070	12.394	9.047	-1.050
500	29.702	48.816	37.763	5.526	12.395	8.675	-0.906
600	32.033	54.437	40.082	8.613	12.396	7.931	-0.690
700	34.363	59.550	42.503	11.933	12.389	7.187	-0.536
800	36.694	64.291	44.934	15.486	12.328	6.447	-0.421
900	39.024	68.747	47.334	19.272	12.085	5.724	-0.332
1000	41.355	72.980	49.689	23.291	11.356	5.049	-0.264
1100	43.689	77.031	51.992	27.543	9.966	4.501	-0.214
1200	46.024	80.932	54.242	32.028	9.362	4.014	-0.175
1200.000	46.024	80.932	54.242	32.028	GLASS <--> LIQUID TRANSITION		
1200.000	46.024	80.932	54.242	32.028			
1300	46.024	84.616	56.438	36.631	10.521	3.521	-0.141
1400	46.024	88.027	58.574	41.233	11.596	2.941	-0.110
1500	46.024	91.202	60.645	45.836	12.588	2.288	-0.080
1600	46.024	94.172	62.649	50.438	13.495	1.571	-0.051
1700	46.024	96.963	64.586	55.040	13.370	0.819	-0.025
1800	46.024	99.593	66.458	59.643	13.776	0.069	-0.002
1809.000	46.024	99.823	66.624	60.057	0.	0.	0.
					DELTA <--> LIQUID		
1900	46.024	102.082	68.258	64.245	0.	0.	0.
2000	46.024	104.442	70.019	68.848	0.	0.	0.
2100	46.024	106.688	71.712	73.450	0.	0.	0.
2200	46.024	108.829	73.351	78.052	0.	0.	0.
2300	46.024	110.875	74.938	82.655	0.	0.	0.
2400	46.024	112.834	76.476	87.257	0.	0.	0.
2500	46.024	114.712	77.968	91.860	0.	0.	0.
2600	46.024	116.517	79.417	96.462	0.	0.	0.
2700	46.024	118.254	80.823	101.064	0.	0.	0.
2800	46.024	119.928	82.190	105.667	0.	0.	0.
2900	46.024	121.543	83.519	110.269	0.	0.	0.
3000	46.024	123.103	84.813	114.872	0.	0.	0.
3100	46.024	124.613	86.073	119.474	0.	0.	0.
3133.345	46.024	125.105	86.483	121.009	0.	0.	0.
					FUGACITY – 1 bar		
3200	46.024	126.074	87.300	124.076	-348.300	7.424	-0.121
3300	46.024	127.490	88.496	128.679	-346.399	18.511	-0.293
3400	46.024	128.864	89.664	133.281	-344.531	29.541	-0.454
3500	46.024	130.198	90.803	137.884	-342.697	40.516	-0.605
3600	46.024	131.495	91.915	142.486	-340.896	51.439	-0.746
3700	46.024	132.756	93.002	147.088	-339.131	62.313	-0.880
3800	46.024	133.983	94.064	151.691	-337.401	73.140	-1.005
3900	46.024	135.179	95.103	156.293	-335.707	83.921	-1.124
4000	46.024	136.344	96.120	160.896	-334.051	94.660	-1.236

Iron (Fe) A_r = 55.847 Iron (Fe) Fe$_t$(cr,l)

CRYSTAL(α–γ–δ)-LIQUID

0	to	1184	K alpha
1184	to	1665	K gamma
1665	to	1809	K delta
above		1809	K liquid

Refer to the individual tables for details.

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

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
		J·K^{-1}·mol^{-1}			kJ·mol^{-1}		
0	0.	0.	INFINITE	-4.507	0.	0.	0.
100	12.101	6.065	46.905	-4.084	0.	0.	0.
200	21.588	17.949	29.524	-2.315	0.	0.	0.
298.15	25.094	27.321	27.321	0.	0.	0.	0.
300	25.140	27.476	27.321	0.046	0.	0.	0.
400	27.386	35.021	28.335	2.674	0.	0.	0.
500	29.702	41.377	30.323	5.527	0.	0.	0.
600	32.049	46.997	32.642	8.613	0.	0.	0.
700	34.602	52.119	35.063	11.939	0.	0.	0.
800	37.949	56.940	37.498	15.553	0.	0.	0.
900	43.095	61.679	39.922	19.582	0.	0.	0.
1000	54.434	66.672	42.342	24.329	0.	0.	0.
1042.000	83.680	69.245	43.372	26.960	C_r LAMBDA MAXIMUM TRANSITION		
1042.000	83.681	69.245	43.372	26.960	0.	0.	0.
1100	46.401	72.062	44.815	29.972			
1184.000	41.422	75.260	46.865	33.619	ALPHA <--> GAMMA TRANSITION		
1184.000	33.882	76.020	46.865	34.519	0.	0.	0.
1200	34.016	76.476	47.257	35.062			
1300	34.853	79.231	49.612	38.505			
1400	35.690	81.845	51.822	42.033			
1500	36.526	84.336	53.907	45.643			
1600	37.363	86.720	55.884	49.338			
1665.000	37.907	88.218	57.117	51.784	GAMMA <--> DELTA TRANSITION		
1665.000	41.112	88.721	57.117	52.621	0.	0.	0.
1700	41.463	89.580	57.776	54.066			
1800	42.468	91.978	59.610	58.263			
1809.000	42.558	92.190	59.772	58.645	DELTA <--> LIQUID TRANSITION		
1809.000	46.024	99.823	59.772	72.452	0.	0.	0.
1900	46.024	102.082	61.744	76.641			
2000	46.024	104.442	63.821	81.243			
2100	46.024	106.688	65.809	85.845			
2200	46.024	108.829	67.716	90.448			
2300	46.024	110.875	69.549	95.050			
2400	46.024	112.833	71.312	99.653			
2500	46.024	114.712	73.010	104.255			
2600	46.024	116.517	74.649	108.857			
2700	46.024	118.254	76.232	113.460			
2800	46.024	119.928	77.763	118.062			
2900	46.024	121.543	79.245	122.665			
3000	46.024	123.103	80.681	127.267			
3100	46.024	124.613	82.074	131.869			
3133.345	46.024	125.105	82.529	133.404	FUGACITY - 1 bar		
3200	46.024	126.074	83.426	136.472	-348.300	7.424	-0.121
3300	46.024	127.490	84.740	141.074	-346.399	18.511	-0.293
3400	46.024	128.864	86.018	145.677	-344.531	29.541	-0.454
3500	46.024	130.198	87.261	150.279	-342.697	40.516	-0.605
3600	46.024	131.495	88.472	154.881	-340.896	51.439	-0.746
3700	46.024	132.756	89.652	159.484	-339.131	62.313	-0.880
3800	46.024	133.983	90.802	164.086	-337.401	73.140	-1.005
3900	46.024	135.179	91.925	168.689	-335.707	83.921	-1.124
4000	46.024	136.344	93.021	173.291	-334.051	94.660	-1.236

Iron, (Fe)   IDEAL GAS $A_r = 55.847$ Iron (Fe)   Fe₁(g)

$I°(Fe, g) = 63480 \pm 500\ cm^{-1}$
$S°(298.15\ K) = 180.49 \pm 0.04\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 413.1 \pm 13\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 415.5 \pm 1.3\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights

State	ϵ, cm⁻¹	g_i
$^5D_4$	0.000	9
$^5D_3$	415.932	7
$^5D_2$	704.004	5
$^5D_1$	888.129	3
$^5D_0$	978.072	1
$^3G_5$	62081.27	5
IP	63480	

Standard State Pressure = $p° = 0.1\ MPa$

Enthalpy Reference Temperature = T_r = 298.15 K

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	
0	0	0.	INFINITE	-6.850	413.127	413.127	INFINITE
100	21.387	154.700	202.317	-4.762	414.794	399.930	-208.902
200	24.362	170.450	182.809	-2.472	415.314	384.814	-100.503
250	25.279	175.995	180.909	-1.228	415.420	377.176	-78.807
298.15	25.675	180.488	180.488	0.	415.471	369.804	-64.788
300	25.682	180.647	180.488	0.048	415.472	369.521	-64.339
350	25.718	184.612	180.801	1.334	415.472	361.862	-54.005
400	25.533	188.036	181.497	2.616	415.412	354.207	-46.255
450	25.233	191.027	182.393	3.885	415.284	346.563	-40.228
500	24.889	193.668	183.391	5.138	415.082	338.937	-35.409
600	24.202	198.144	185.490	7.592	414.451	323.762	-28.186
700	23.610	201.829	187.559	9.982	413.514	308.717	-23.037
800	23.113	204.949	189.551	12.318	412.236	293.829	-19.185
900	22.763	207.651	191.416	14.612	410.501	279.127	-16.200
1000	22.488	210.035	193.161	16.874	408.016	264.653	-13.824
1100	22.297	212.168	194.793	19.113	404.612	250.495	-11.895
1200	22.183	214.103	196.323	21.336	401.745	236.592	-10.299
1300	22.156	215.876	197.760	23.551	400.517	222.879	-8.955
1400	22.231	217.517	199.113	25.766	399.204	209.263	-7.808
1500	22.356	219.048	200.392	27.984	397.812	195.744	-6.816
1600	22.523	220.487	201.603	30.213	396.347	182.320	-5.952
1700	22.726	221.847	202.754	32.457	393.862	169.009	-5.193
1800	22.958	223.140	203.851	34.719	391.928	155.837	-4.522
1900	23.213	224.374	204.899	37.003	375.834	143.477	-3.944
2000	23.485	225.558	205.903	39.312	373.540	131.308	-3.429
2100	23.771	226.698	206.866	41.646	371.272	119.252	-2.966
2200	24.065	227.797	207.793	44.009	369.033	107.303	-2.548
2300	24.365	228.860	208.683	46.401	366.822	95.456	-2.168
2400	24.669	229.890	209.548	48.822	364.641	83.705	-1.822
2500	24.976	230.891	210.381	51.274	362.490	72.043	-1.505
2600	25.284	231.865	211.189	53.756	360.370	60.467	-1.215
2700	25.594	232.813	211.973	56.269	358.280	48.972	-0.947
2800	25.905	233.738	212.733	58.813	356.222	37.554	-0.701
2900	26.219	234.642	213.473	61.388	354.195	26.209	-0.472
3000	26.536	235.525	214.194	63.994	352.198	14.933	-0.260
3100	26.674	236.390	214.896	66.632	350.234	3.724	-0.063
3133.345	26.856	236.674	215.126	67.518	0.	0.	—
3200	27.181	237.237	215.581	69.301	0.	0.	—
3300	27.511	238.069	216.250	72.003	0.	0.	—
3400	27.848	238.885	216.903	74.738	0.	0.	—
3500	28.192	239.687	217.543	77.506	0.	0.	—
3600	28.544	240.477	218.169	80.308	0.	0.	—
3700	28.905	241.254	218.783	83.144	0.	0.	—
3800	29.274	242.020	219.384	86.017	0.	0.	—
3900	29.654	242.776	219.974	88.925	0.	0.	—
4000	30.043	243.521	220.554	91.872	0.	0.	—
4100	30.442	244.258	221.123	94.856	0.	0.	—
4200	30.851	244.987	221.682	97.881	0.	0.	—
4300	31.270	245.708	222.233	100.945	0.	0.	—
4400	31.701	246.422	222.774	104.051	0.	0.	—
4500	32.142	247.130	223.308	107.200	0.	0.	—
4600	32.594	247.831	223.833	110.392	0.	0.	—
4700	33.058	248.527	224.351	113.628	0.	0.	—
4800	33.533	249.219	224.862	116.911	0.	0.	—
4900	34.022	249.905	225.366	120.240	0.	0.	—
5000	34.524	250.587	225.864	123.618	0.	0.	—
5100	35.040	251.266	226.355	127.045	0.	0.	—
5200	35.572	251.941	226.841	130.523	0.	0.	—
5300	36.120	252.614	227.321	134.054	0.	0.	—
5400	36.687	253.284	227.795	137.638	0.	0.	—
5500	37.274	253.952	228.265	141.278	0.	0.	—
5600	37.882	254.618	228.729	144.976	0.	0.	—
5700	38.513	255.283	229.189	148.734	0.	0.	—
5800	39.170	255.947	229.643	152.553	0.	0.	—
5900	39.853	256.611	230.097	156.437	0.	0.	—
6000		257.275	230.544	160.388	0.	0.	—

FUGACITY = 1 bar

Enthalpy of Formation

The sublimation and vaporization studies on iron are too numerous to tabulate. A current literature survey by Hultgren yielded approximately thirty investigations.[1] As in Hultgren,[2] we adopt $\Delta_f H°(Fe, g, 298.15\ K) = 99.3 \pm 0.3\ kcal\ mol^{-1}$ based on the studies of Morris et al.[3] and Myles and Aldred.[4] A complete listing of all vapor pressure studies is available on request. Many of the more recent studies do not provide sufficient information to enable calculation of enthalpy of formation values via the 2nd and 3rd law approach.

Our 2nd and 3rd law analyses of the vaporization data of Morris et al.[3] and the sublimation data of Myles and Aldred[4] are given below.

Source	Data Points	T/K	$\Delta_f H°$(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
Fe(l) → Fe(g)	21	1812–1891	96.8 ± 1.1	96.5 ± 0.1	0.1 ± 6	99.5
Fe(γ) → Fe(g)	eqn	1450–1650	98.1	97.1	-0.6	99.0

Heat Capacity and Entropy

The electronic energy levels are given in the compilation by Reader and Sugar.[5] Although we have only listed the ground state, the lowest four excited states, the highest observed excited state, and the ionization limit for Fe(g), all levels listed by Reader and Sugar[5] as well as estimated missing levels, are used in the calculations. The observed levels are too numerous to list completely. Our calculations indicate that for Fe(g) the thermochemical functions are independent of the estimated missing levels (for $n = 4, 5, 6, 7$) and the cutoff procedure up to 3500 K. The Gibbs energy function is essentially unaffected up to 5200 K. The reported uncertainty in $S°(298.15\ K)$ is due to uncertainties in the relative atomic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states and utilization of proper fill and cutoff procedures.[6] In fact, the inclusion of some higher states ($n = 4, 5, 6, 7$) and consideration of various cut-off procedures leads to calculational differences in the Gibbs energy function of roughly $0.1\ cal \cdot K^{-1} \cdot mol^{-1}$ or greater at temperatures in excess of 8000 K.

References

[1] R. Hultgren, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, personal communication.

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[4] K. M. Myles and A. T. Aldred, J. Phys. Chem. 68, 64 (1964).

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Fe₁(g)

Iron, Ion (Fe⁺)   IDEAL GAS $M_r = 55.84645$ Fe⁺(g)

$IP(Fe^+, g) = 130563 \pm 10$ cm⁻¹
$S°(298.15\ K) = 181.86 \pm 0.05$ J·K⁻¹·mol⁻¹

$\Delta_f H°(0\ K) = 1172.52 \pm 7.5$ kJ·mol⁻¹
$\Delta_f H°(298.15\ K) = [1181.144]$ kJ·mol⁻¹

Electronic Levels and Quantum Weights

State	ε_i, cm⁻¹	g_i
$^6D_{9/2}$	0.000	10
$^6D_{7/2}$	384.790	8
$^6D_{5/2}$	667.683	6
$^6D_{3/2}$	862.613	4
$^6D_{1/2}$	977.053	2
⋮	⋮	⋮

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
		J·K⁻¹·mol⁻¹			kJ·mol⁻¹		
0	0	0	INFINITE	−6.936	1172.517		
100	21.618	155.635	204.058	−4.842			
200	24.813	171.652	184.215	−2.512			
250	25.689	177.294	182.284	−1.248			
298.15	26.068	181.857	181.857	0	1181.144	1128.814	−197.764
300	26.075	182.018	181.857	0.048	1181.184	1128.489	−196.487
350	26.163	186.047	182.175	1.355	1182.244	1119.622	−167.094
400	26.112	189.538	182.882	2.662	1183.249	1110.507	−145.030
450	26.018	192.608	183.796	3.966	1184.194	1101.470	−127.855
500	25.931	195.345	184.816	5.264	1185.076	1092.230	−114.104
600	25.830	200.062	186.976	7.851	1186.656	1073.508	−93.457
700	25.802	204.041	189.137	10.433	1187.990	1054.541	−78.691
800	25.786	207.485	191.220	13.012	1189.034	1035.402	−67.605
900	25.744	210.521	193.199	15.589	1189.661	1016.155	−58.976
1000	25.661	213.229	195.069	18.160	1189.562	996.872	−52.071
1100	25.539	215.669	196.833	20.720	1188.559	977.666	−46.423
1200	25.390	217.885	198.497	23.266	1188.094	958.495	−41.722
1300	25.225	219.911	200.067	25.797	1189.260	939.314	−37.742
1400	25.054	221.774	201.552	28.311	1190.325	920.047	−34.327
1500	24.885	223.497	202.958	30.808	1191.290	900.707	−31.365
1600	24.726	225.098	204.293	33.289	1192.155	881.306	−28.772
1700	24.579	226.592	205.561	35.754	1191.970	861.872	−26.482
1800	24.447	227.993	206.769	38.205	1192.303	842.445	−24.447
1900	24.330	229.312	207.921	40.644	1178.443	823.703	−22.645
2000	24.229	230.557	209.022	43.071	1178.347	805.035	−21.025
2100	24.144	231.737	210.076	45.490	1178.242	786.372	−19.550
2200	24.074	232.859	211.086	47.901	1178.129	767.714	−18.228
2300	24.018	233.928	212.056	50.305	1178.009	749.062	−17.012
2400	23.975	234.949	212.989	52.705	1177.885	730.415	−15.897
2500	23.945	235.927	213.887	55.101	1177.757	711.773	−14.872
2600	23.927	236.866	214.753	57.494	1177.627	693.136	−13.925
2700	23.920	237.769	215.588	59.886	1177.495	674.504	−13.049
2800	23.925	238.639	216.396	62.278	1177.363	655.877	−12.236
2900	23.940	239.478	217.178	64.672	1177.233	637.255	−11.478
3000	23.966	240.290	217.935	67.067	1177.104	618.637	−10.771
3100	24.002	241.077	218.669	69.465	1176.979	600.024	−10.110
3200	24.049	241.840	219.381	71.868	828.558	588.558	−9.612
3300	24.104	242.580	220.073	74.275	830.342	581.319	−9.202
3400	24.170	243.301	220.745	76.689	832.100	573.747	−8.815
3500	24.245	244.003	221.400	79.110	833.831	566.123	−8.449
3600	24.329	244.687	222.037	81.538	835.536	558.450	−8.103
3700	24.423	245.355	222.658	83.976	837.216	550.730	−7.775
3800	24.525	246.007	223.264	86.423	838.869	542.965	−7.464
3900	24.636	246.646	223.856	88.881	840.497	535.156	−7.168
4000	24.756	247.271	224.433	91.351	842.099	527.307	−6.886
4100	24.883	247.884	224.998	93.833	843.675	519.417	−6.617
4200	25.018	248.485	225.550	96.328	845.224	511.490	−6.361
4300	25.161	249.075	226.090	98.836	846.747	503.526	−6.117
4400	25.310	249.656	226.619	101.360	848.243	495.526	−5.883
4500	25.467	250.226	227.137	103.899	849.712	487.493	−5.659
4600	25.629	250.788	227.646	106.453	851.154	479.428	−5.444
4700	25.797	251.341	228.144	109.025	852.567	471.332	−5.238
4800	25.970	251.885	228.633	111.613	853.951	463.206	−5.041
4900	26.149	252.423	229.113	114.219	855.306	455.051	−4.851
5000	26.331	252.953	229.584	116.843	856.631	446.869	−4.668
5100	26.518	253.476	230.048	119.485	857.925	438.661	−4.493
5200	26.708	253.993	230.503	122.147	859.187	430.428	−4.324
5300	26.901	254.503	230.951	124.827	860.415	422.171	−4.161
5400	27.096	255.008	231.392	127.527	861.609	413.891	−4.004
5500	27.293	255.507	231.826	130.246	862.767	405.589	−3.852
5600	27.493	256.001	232.253	132.985	863.887	397.266	−3.706
5700	27.693	256.489	232.674	135.745	864.967	388.924	−3.564
5800	27.894	256.972	233.089	138.524	866.006	380.564	−3.427
5900	28.095	257.451	233.498	141.324	867.000	372.185	−3.295
6000	28.297	257.925	233.901	144.143	867.947	363.791	−3.167

Enthalpy of Formation

$\Delta_f H°(Fe^+, g, 0\ K)$ is calculated from $\Delta_f H°(Fe, g, 0\ K)$[1] using the spectroscopic value of IP(Fe) = 63480 ± 500 cm⁻¹ (759.390 ± 5.98 kJ·mol⁻¹) from Corliss and Sugar.[2] The ionization limit is converted from cm⁻¹ to kJ·mol⁻¹ using the factor, 1 cm⁻¹ = 0.01196266 kJ·mol⁻¹, which is derived from the 1973 CODATA fundamental constants.[3] Rosenstock et al.[4] and Levin and Lias[5] have summarized additional ionization and appearance potential data.

$\Delta_f H°(Fe^+, g, 298.15\ K)$ is calculated from $\Delta_f H°(Fe, g, 0\ K)$ by using IP(Fe) with JANAF[1] enthalpies, $H°(0\ K)-H°(298.15\ K)$, for Fe(g), Fe⁺(g), and e⁻(ref). $\Delta_f H°(Fe \to Fe^+ + e^-, 298.15\ K)$ 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 five levels for Fe⁺(g), all levels listed by Corliss and Sugar[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 Fe⁺(g), the thermodynamic functions are independent of the estimated missing levels (for n=4), the cut-off procedure, and the inclusion of n=5 levels up to 6000 K; the Gibbs energy function showing no significant variations at this temperature. The reported uncertainty in S°(298.15 K) is due to uncertainties in the relative ionic mass, and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states (n>5), and use of different fill and cut-off procedures.[6]

References

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Iron, Ion (Fe⁺)   Fe⁺(g)

Iron, Ion (Fe⁻)   IDEAL GAS $M_r = 55.84755$ Iron, Ion (Fe⁻)   Fe⁻(g)

$EA(\mathrm{Fe}, g) = 0.163 \pm 0.035$ eV

$S°(298\ 15\ \mathrm{K}) = 180.198 \pm 0.005$ J·K⁻¹·mol⁻¹

$\Delta_f H°(0\ \mathrm{K}) = 397\ 400 \pm 4\ 4$ kJ mol⁻¹

$\Delta_f H°(298\ 15\ \mathrm{K}) = [393\ 338]$ kJ·mol⁻¹

Electronic Levels and Quantum Weights

State	ϵ_i, cm⁻¹	g_i
$^4F_{9/2}$	0	10
$^4F_{7/2}$	540	8
$^4F_{5/2}$	930	6
$^4F_{3/2}$	1200	4

T/K		J·K⁻¹·mol⁻¹			kJ·mol⁻¹		
	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
0	0.	0	INFINITE	-6.642	397.400		
100	20.957	155.485	201.095	-4.561			
200	23.092	170.579	182.433	-2.371			
250	24.226	175.858	180.606	-1.187			
298.15	25.023	180.198	180.198	0.	393.338	354.013	-62.002
300	25.047	180.353	180.198	0.046	393.300	353.769	-61.597
350	25.536	184.254	180.505	1.312	392.240	347.264	-51.826
400	25.748	187.681	181.193	2.595	391.142	340.913	-44.519
450	25.758	190.716	182.085	3.884	389.994	334.703	-38.851
500	25.632	193.424	183.086	5.169	388.784	328.624	-34.331
600	25.172	198.059	185.208	7.710	386.162	316.833	-27.583
700	24.627	201.899	187.327	10.201	383.247	305.505	-22.797
800	24.108	205.153	189.357	12.637	379.990	294.616	-19.236
900	23.652	207.965	191.272	15.024	376.271	284.162	-16.492
1000	23.264	210.437	193.067	17.370	371.790	274.158	-14.321
1100	22.938	212.638	194.748	19.679	366.378	264.671	-12.568
1200	22.666	214.622	196.323	21.959	361.489	255.621	-11.127
1300	22.438	216.427	197.801	24.214	358.222	246.930	-9.922
1400	22.246	218.083	199.191	26.448	354.851	238.495	-8.898
1500	22.084	219.612	200.502	28.664	351.377	230.305	-8.020
1600	21.946	221.033	201.742	30.865	347.806	222.349	-7.259
1700	21.829	222.360	202.916	33.054	343.188	214.639	-6.595
1800	21.727	223.604	204.031	35.232	339.090	207.195	-6.013
1900	21.640	224.777	205.092	37.400	320.802	200.683	-5.517
2000	21.563	225.883	206.105	39.560	316.281	194.478	-5.079
2100	21.496	226.935	207.072	41.713	311.753	188.499	-4.689
2200	21.438	227.934	207.997	43.860	307.218	182.736	-4.339
2300	21.386	228.885	208.885	46.001	302.678	177.179	-4.024
2400	21.340	229.795	209.738	48.137	298.134	171.820	-3.740
2500	21.299	230.665	210.557	50.269	293.585	166.651	-3.482
2600	21.262	231.500	211.347	52.397	289.032	161.663	-3.248
2700	21.229	232.301	212.108	54.521	284.475	156.851	-3.034
2800	21.199	233.073	212.843	56.643	279.916	152.208	-2.839
2900	21.173	233.816	213.554	58.761	275.353	147.727	-2.661
3000	21.148	234.534	214.241	60.877	270.788	143.404	-2.497
3100	21.126	235.227	214.907	62.991	266.221	139.233	-2.346
3200	21.106	235.897	215.553	65.103	-86.649	142.634	-2.328
3300	21.088	236.546	216.179	67.212	-89.319	149.840	-2.372
3400	21.071	237.176	216.787	69.320	-92.024	157.128	-2.414
3500	21.055	237.786	217.427	71.427	-94.765	164.495	-2.455
3600	21.041	238.379	217.954	73.531	-97.540	171.942	-2.495
3700	21.028	238.955	218.514	75.635	-100.352	179.466	-2.534
3800	21.015	239.516	219.059	77.737	-103.201	187.067	-2.571
3900	21.004	240.062	219.590	79.838	-106.088	194.743	-2.608
4000	20.993	240.593	220.109	81.938	-109.013	202.494	-2.644
4100	20.984	241.112	220.615	84.037	-111.977	210.318	-2.679
4200	20.975	241.617	221.109	86.134	-114.982	218.215	-2.714
4300	20.966	242.111	221.592	88.232	-118.028	226.184	-2.748
4400	20.958	242.593	222.063	90.328	-121.116	234.225	-2.781
4500	20.951	243.063	222.523	92.423	-124.248	242.336	-2.813
4600	20.944	243.524	222.976	94.518	-127.424	250.517	-2.845
4700	20.937	243.974	223.418	96.612	-130.645	258.768	-2.876
4800	20.931	244.415	223.851	98.705	-133.913	267.088	-2.907
4900	20.925	244.846	224.275	100.798	-137.228	275.476	-2.937
5000	20.920	245.269	224.691	102.890	-140.592	283.933	-2.966
5100	20.915	245.683	225.099	104.982	-144.006	292.457	-2.995
5200	20.910	246.089	225.498	107.073	-147.472	301.049	-3.024
5300	20.905	246.488	225.891	109.164	-150.990	309.708	-3.052
5400	20.901	246.878	226.276	111.255	-154.563	318.434	-3.080
5500	20.897	247.262	226.654	113.344	-158.191	327.226	-3.108
5600	20.893	247.638	227.025	115.434	-161.878	336.085	-3.135
5700	20.890	248.008	227.390	117.523	-165.626	345.011	-3.162
5800	20.886	248.371	227.749	119.612	-169.435	354.003	-3.188
5900	20.883	248.728	228.101	121.700	-173.309	363.060	-3.214
6000	20.880	249.079	228.448	123.788	-177.250	372.184	-3.240

Enthalpy of Formation

$\Delta_f H°(\mathrm{Fe^-}, g, 0\ \mathrm{K})$ is calculated from $\Delta_f H°(\mathrm{Fe}, g, 0\ \mathrm{K})$[1] using the adopted electron affinity of $EA(\mathrm{Fe}) = 0\ 163 \pm 0\ 035$ eV $(15,727 \pm 3,377$ kJ mol⁻¹). This value, recommended by Hotop and Lineberger,[2] is based on a laser photodetachment electron spectrometry study.[3] Additional information on Fe⁻(ref) may be obtained in the critical discussions of Hotop and Lineberger,[2,4] Rosenstock et al.[5] and Massey.[6] $\Delta_f H°(\mathrm{Fe^-}, g, 298.15\ \mathrm{K})$ is obtained from $\Delta_f H°(\mathrm{Fe}, g, 0\ \mathrm{K})$ by using $EA(\mathrm{Fe})$ with JANAF[1] enthalpies, $H°(0\ \mathrm{K}) - H°(298.15\ \mathrm{K})$, or Fe⁻(ref), Fe(g), and e⁻(ref). $\Delta_f H°(\mathrm{Fe^-} \to \mathrm{Fe} + \mathrm{e^-}, 298.15\ \mathrm{K})$ differs from a room-temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock et al.[5] $\Delta_f H°(298.15\ \mathrm{K})$ 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 ground state electronic configuration for Fe⁻(ref) is given by Hotop and Lineberger[2,4] and Rosenstock et al.[5] The fine structure separations in the ground state have been calculated by an isoelectronic extrapolation of ratios of fine structure separations.[7]

References

[1]JANAF Thermochemical Tables: Fe(g), 3-31-78; e⁻(ref), 3-31-82.

[2]H. Hotop and W. C. Lineberger, J. Phys. Chem. Ref. Data, 14, 731 (1985).

[3]P. C. Engelking and W. C. Lineberger, Phys. Rev. A 19, 149 (1979).

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[6]H. S. W. Massey, "Negative Ions," 3rd ed., Cambridge University Press, Cambridge, (1976).

[7]C. S. Feigerle, R. R. Corderman, S. V. Babashev, and W. C. Lineberger, J. Chem. Phys. 74, 1580 (1981).

Iron Hydroxide (Fe(OH)₂) — CRYSTAL

$M_r = 89.86168$ Iron Hydroxide (Fe(OH)₂)   Fe₁H₂O₂(cr)

$S°(298.15 K) = [87.864 \pm 8.4]$ J·K⁻¹·mol⁻¹
T_{fus} = Unknown

$\Delta_f H°(0 K)$ = Unknown
$\Delta_f H°(298.15 K) = -574.04 \pm 2.9$ kJ·mol⁻¹
$\Delta_{sub} H°$ = Unknown

T/K	C°p	S°	-[G°-H°(Tr)]/T	H°-H°(Tr)	ΔfH°	ΔfG°	log Kf
		J·K⁻¹·mol⁻¹			kJ·mol⁻¹		
0							
100							
200							
298.15	97.069	87.864	87.864	0.	-574.045	-491.969	86.191
300	97.152	88.465	87.866	0.180	-574.019	-491.460	85.571
400	102.090	117.096	91.736	10.144	-572.560	-464.155	60.612
500	106.776	140.383	99.206	20.589	-570.950	-437.238	45.678
600	111.294	160.255	107.764	31.495	-569.218	-410.656	35.751
700	115.478	177.734	116.535	42.839	-567.392	-384.373	28.682
800	118.951	193.391	125.181	54.568	-565.567	-358.353	23.398
900	121.545	207.559	133.559	66.599	-563.945	-332.552	19.301
1000	123.386	220.466	141.614	78.852	-562.905	-306.906	16.031
1100	124.516	232.283	149.328	91.251	-562.696	-281.301	13.358
1200	125.102	243.145	156.699	103.735	-561.930	-255.773	11.134
1300	125.353	253.170	163.740	116.259	-559.553	-230.357	9.256
1400	125.436	262.462	170.463	128.799	-557.318	-205.119	7.653
1500	125.520	271.119	176.889	141.346	-555.230	-180.036	6.269

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

Enthalpy of Formation

The enthalpy of combustion of Fe(OH)₂(cr), according to the chemical reaction Fe(OH)₂(cr) + 1/4 O₂(g) = 1/2 Fe₂O₃(cr) + H₂O(l) was determined to be -29.8 ± 0.65 kcal·mol⁻¹ by Fricke and Rihl.[1] From these data the adopted enthalpy of formation, $\Delta_f H°$(298.15 K), was evaluated to be -137.2 ± 0.7 kcal·mol⁻¹.

The enthalpy changes for the following three reactions were determined by Thomsen.[2]

Reaction	ΔrH°(291 K), kcal·mol⁻¹
FeCl₂(cr) = FeCl₂ (400 H₂O)	-17.9
FeCl₂(200 H₂O) + H₂SO₄(200 H₂O) = FeSO₄(200 H₂O) + 2 HCl(100 H₂O)	-3.6
FeSO₄(aq) + 2 KOH(aq) = Fe(OH)₂(cr) + K₂SO₄(aq)	-6.34

Using $\Delta_f H°$(298.15 K) = -81.7 kcal·mol⁻¹ for FeCl₂(cr) and those for the other compounds in aqueous solution (assuming aq. = 200 H₂O in Reaction 3) obtained from Wagman et al.[3] the enthalpy of formation at 298.15 K for Fe(OH)₂(cr) was derived as -135.8 kcal·mol⁻¹ which agrees reasonably with the adopted value.

Heat Capacity and Entropy

The heat capacities, 298.15-700 K and S°(298.15 K) were estimated by comparison with those for FeCl₂(cr), CaCl₂(cr) and Ca(OH)₂(cr). The C°p values above 700 K were obtained by graphical extrapolation of the C°p curve plotted using the above C°p values.

Sublimation Data

The value of $\Delta_{sub} H°$(298.15 K) was calculated as the difference between $\Delta_f H°$(298.15 K) for Fe(OH)₂(g) and Fe(OH)₂(cr).

References

[1] R. Fricke and S. Rihl, Z. anorg. allg. Chem. 251, 414 (1943).
[2] J. Thomsen, "Thermochemische Untersuchungen," Barth, Leipzig, 1882-1886.
[3] U. S. Nat. Bur. Stand. Tech. Note 270-1, (1965).

Iron Hydroxide (Fe(OH)₂)   Fe₁H₂O₂(cr)

Iron Hydroxide (Fe(OH)₂)   IDEAL GAS M_r = 89.86168   **Iron Hydroxide (Fe(OH)₂)**   Fe₁H₂O₂(g)

$S°(298\ 15\ K) = [283.088]\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = [-323.09 \pm 2.1]\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = [-330.54 \pm 2.1]\ kJ\cdot mol^{-1}$

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	.000	.000	INFINITE	-14.209	-323.088	-323.088	INFINITE
100	36.766	227.041	335.221	-10.818	-326.023	-320.717	167.526
200	55.199	257.765	289.157	-6.278	-328.857	-314.241	82.071
250	64.437	271.106	284.228	-3.280	-329.851	-310.466	64.868
298.15	71.504	283.088	283.088	.000	-330.536	-306.666	53.727
300	71.738	283.531	283.089	.133	-330.558	-306.518	53.370
350	77.115	295.015	283.984	3.861	-331.041	-302.471	45.141
400	81.011	305.581	286.032	7.819	-331.376	-298.365	38.962
450	83.894	315.297	288.752	11.945	-331.625	-294.223	34.153
500	86.129	324.256	291.860	16.198	-331.831	-290.056	30.302
600	89.528	340.275	298.626	24.989	-332.215	-281.665	24.521
700	92.212	354.284	305.598	34.080	-332.642	-273.207	20.387
800	94.509	366.751	312.477	43.419	-333.207	-264.681	17.282
900	95.515	378.001	319.142	52.973	-334.063	-256.067	14.862
1000	98.263	388.262	325.549	62.714	-335.535	-247.331	12.919
1100	99.773	397.700	331.685	72.617	-337.821	-238.385	11.320
1200	101.068	406.439	337.554	82.661	-339.495	-229.290	9.981
1300	102.172	414.573	343.170	92.825	-339.479	-220.108	8.844
1400	103.108	422.180	348.545	103.090	-339.518	-210.924	7.870
1500	103.901	429.322	353.694	113.441	-339.627	-201.736	7.025
1600	104.571	436.049	358.633	123.866	-339.815	-192.537	6.286
1700	105.137	442.406	363.376	134.352	-341.042	-183.306	5.632
1800	105.614	448.430	367.935	144.890	-341.750	-174.007	5.050
1900	106.018	454.151	372.323	155.473	-356.658	-163.965	4.508
2000	106.360	459.598	376.552	166.092	-357.814	-153.793	4.017
2100	106.650	464.795	380.631	176.743	-358.996	-143.563	3.571
2200	106.895	469.762	384.571	187.420	-360.208	-133.275	3.164
2300	107.104	474.518	388.379	198.121	-361.452	-122.933	2.792
2400	107.281	479.080	392.064	208.840	-362.729	-112.536	2.449
2500	107.432	483.463	395.633	219.576	-364.040	-102.084	2.133
2600	107.561	487.679	399.092	230.326	-365.387	-91.579	1.840
2700	107.671	491.741	402.449	241.088	-366.769	-81.022	1.567
2800	107.765	495.658	405.708	251.860	-368.187	-70.412	1.314
2900	107.845	499.441	408.876	262.640	-369.640	-59.753	1.076
3000	107.914	503.098	411.956	273.428	-371.129	-49.041	.854
3100	107.973	506.638	414.953	284.223	-372.652	-38.280	.645
3200	108.023	510.067	417.872	295.022	-722.510	-20.046	.327
3300	108.066	513.391	420.717	305.827	-722.202	1.901	-.030
3400	108.103	516.618	423.490	316.635	-721.960	23.841	-.366
3500	108.134	519.752	426.196	327.447	-721.785	45.773	-.683
3600	108.161	522.799	428.837	338.262	-721.676	67.702	-.982
3700	108.184	525.763	431.417	349.079	-721.634	89.628	-1.265
3800	108.203	528.648	433.938	359.899	-721.660	111.555	-1.533
3900	108.220	531.459	436.402	370.720	-721.753	133.483	-1.788
4000	108.234	534.199	438.813	381.543	-721.915	155.413	-2.029
4100	108.245	536.872	441.172	392.367	-722.145	177.349	-2.259
4200	108.255	539.480	443.482	403.192	-722.444	199.292	-2.479
4300	108.263	542.028	445.744	414.018	-722.814	221.242	-2.688
4400	108.270	544.517	447.961	424.844	-723.255	243.201	-2.887
4500	108.275	546.950	450.134	435.671	-723.767	265.171	-3.078
4600	108.279	549.330	452.265	446.499	-724.352	287.154	-3.261
4700	108.284	551.658	454.355	457.327	-725.010	309.150	-3.436
4800	108.285	553.938	456.406	468.156	-725.743	331.162	-3.604
4900	108.287	556.171	458.419	478.984	-726.551	353.189	-3.765
5000	108.288	558.358	460.396	489.813	-727.436	375.234	-3.920
5100	108.289	560.503	462.338	500.642	-728.399	397.297	-4.069
5200	108.289	562.606	464.246	511.471	-729.442	419.378	-4.213
5300	108.288	564.668	466.121	522.300	-730.565	441.483	-4.351
5400	108.288	566.692	467.965	533.128	-731.770	463.607	-4.485
5500	108.287	568.679	469.778	543.957	-733.060	485.755	-4.613
5600	108.286	570.631	471.562	554.786	-734.436	507.929	-4.738
5700	108.284	572.547	473.317	565.614	-735.900	530.126	-4.858
5800	108.283	574.430	475.044	576.443	-737.455	552.352	-4.974
5900	108.281	576.281	476.744	587.271	-739.103	574.601	-5.087
6000	108.279	578.101	478.418	598.099	-740.847	596.883	-5.196

Electronic Levels and Quantum Weights

ϵ_i, cm⁻¹	g_i
0	[5]
[700]	[10]
[2500]	[5]
[4000]	[5]

Vibrational Frequencies and Degeneracies

ν_i, cm⁻¹

[2300](1)	[450](1)	[800](1)
[750](1)	[320](1)	[700](1)
[400](1)	[2600](1)	[570](1)

Point Group: [C₂ᵥ] $\sigma = 2$
Bond Distances: Fe-O = [1.8] Å   O-H = [0.96] Å
Bond Angles: O-Fe-O = [180]°   Fe-O-H = [105]°
Product of the Moments of Inertia: $I_A I_B I_C = [9.90391 \times 10^{-115}]$ g³·cm⁶

Enthalpy of Formation

The equilibrium constants, at temperatures between 1300 and 1460°C, for the chemical reaction Fe(cr) + 2 H₂O(g) = Fe(OH)₂(g) + H₂(g) were determined by Belton and Richardson.[1] Using these data, the enthalpy change, $\Delta_r H°$ (298.15 K), of the reaction is evaluated to be 35.53 ± 3.0 and 36.57 kcal·mol⁻¹ by the 2nd and 3rd law method, respectively. Based on the 3rd law value for $\Delta_r H°$(298 15 K), the enthalpy of formation, $\Delta_f H°$(Fe(OH)₂, g, 298.15 K), is calculated to be -79 ± 0.5 kcal mol⁻¹.

Heat Capacity and Entropy

The molecular structure is assumed to be the same as that for B(OH)₂(g). The Fe-O bond distance is taken from FeO(g). The O-H bond distance and Fe-O-H bond angle are estimated from those for H₂O(g). The vibrational frequencies, and electronic levels and quantum weights are obtained by comparison with those for B(OH)₂(g) and FeCl₂(g), respectively. These values are adjusted to give reasonable 2nd and 3rd law agreements. The principal moments of inertia are: $I_A = 0.2814 \times 10^{-39}$, $I_B = 18.6208\ 10^{-39}$, and $I_C = 18.9022 \times 10^{-39}$ g·cm².

Reference

[1] G. R. Belton and F. D. Richardson, Trans. Faraday Soc. 58, 1562 (1962).

Iron Hydroxide (Fe(OH)₃) CRYSTAL $M_r = 106.86902$ Iron Hydroxide (Fe(OH)₃) Fe₁H₃O₃(cr)

$S°(298.15\ K) = [104.600 \pm 8\ 4]\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = Unknown$

$T_{fus} = Unknown$

$\Delta_f H°(298.15\ K) = -832.62 \pm 12.6\ kJ \cdot mol^{-1}$

$\Delta_{fus} H° = Unknown$

Enthalpy of Formation

Schindler et al.[1] investigated the solubility of aged Fe(OH)₃ precipitates by determining the Fe^{3+} and H^+ ion concentration of solution in contact with the solid phase. The ion concentration was measured by the EMF-method at the constant ionic strength 3M NaClO₄(solution). The precipitates were investigated by X-ray and electron microscope methods. The equilibrium constant was derived as $\log [Fe^{3+}][H^+]^3 = \log K = 3.55 \pm 0.1$ for amorphous inactive hydroxide at 25°C. From these data the quantity $\log Ks = -39.1 \pm 0.2$ was evaluated where Ks is the solubility product of Fe(OH)₃. The Gibbs energy change, $\Delta_f G°(298.15\ K)$, of the reaction Fe(OH)₃(cr) = Fe³⁺(aq) + 3 OH⁻(aq) was calculated to be $53.34 \pm 0.27\ kcal \cdot mol^{-1}$. Using $S°(298.15\ K) = -70.1$ and 2.57 cal·K⁻¹·mol⁻¹ for Fe³⁺(aq) and OH⁻(aq), respectively, and an estimated S°(Fe(OH)₃), cr, 298.15 K) = 25 cal·K⁻¹·mol⁻¹, the enthalpy change, $\Delta_f H°(298.15\ K)$, cr, 298.15 K), the enthalpy change, $\Delta_f H°(298.15\ K)$ of the reaction is calculated to be 22.69 kcal·mol⁻¹, according to the relationship $\Delta H = \Delta F + T\Delta S$ The entropy values for Fe³⁺ and OH⁻ ions, were obtained from[2] and[3] respectively. Based on $\Delta_f H°(Fe^{3+}$, aq, 298.15 K) = -11.4 and $\Delta_f H°(OH^-$, aq, 298.15 K) = -54.97 kcal·mol⁻¹, taken from the same sources, the enthalpy of formation, $\Delta_f H°(298.15\ K)$, for Fe(OH)₃(cr) was evaluated to be -199 ± 3 kcal·mol⁻¹, which was adopted here.

The divergent values for solubility product (SP) of Fe(OH)₃ found in the literature may be due, not only to the various forms of precipitate but also to the tendency to form colloidal solutions. The SP values for Fe(OH)₃ were also reported by Evans and Pryor[4] Kriukor and Awsejewitsch[5] Ruff and Hirsch[6] Britton[7] and Jellinek and Gorden.[8]

The enthalpy changes, $\Delta_f H°(291\ K)$, for the reactions: (1) FeCl₃(aq) + 3NaOH(aq) = Fe(OH)₃(cr) + 3NaCl(aq) and (2) FeCl₃(cr) = FeCl₃(aq) were determined to be -24.50 and -31.68 kcal·mol⁻¹, respectively by Thomsen.[9] Assuming the aqueous solutions all contain 200 mol of H₂O, the enthalpy of formation, $\Delta_f H°(298.15\ K)$, for Fe(OH)₃ was calculated as -196.9 kcal·mol⁻¹ from Reaction (1) and (2). The $\Delta_f H°(298.15\ K)$ values for NaOH(aq) and NaCl(aq) were obtained from Parker[10] and JANAF $\Delta_f H°(298.15\ K)$ values for NaOH(cr) and NaCl(cr).

Heat Capacity and Entropy

The heat capacities, 298 15-1000 K, were estimated by comparison with those for B₂O₃(cr), Fe₂O₃(cr) and B(OH)₃(cr). The C_p° values above 1000 K were obtained by graphical extrapolation. The S°(Fe(OH)₃, cr, 298.15 K) value was estimated by comparison with that for B(OH)₃(cr).

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[8]Jellinek and Gorden, Z. Phys. Chem. 112, 207 (1924).
[9]J. Thomsen, "Thermochemische Untersuchungen," Barth, Leipzig, 1882–1886.
[10]V. B. Parker, NSRDS NBS 2, (1965).

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

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	
0							
100							
200							
298.15	101.671	104.600	104.600	0.	-832.616	-705.467	123.595
300	102.090	105.230	104.602	0.188	-832.636	-704.678	122.695
400	117.989	136.877	108.809	11.227	-833.040	-661.930	86.439
500	129.704	164.480	117.242	23.619	-832.474	-619.202	64.688
600	140.582	189.140	127.205	37.161	-831.150	-576.661	50.203
700	148.114	211.387	137.669	51.603	-829.323	-534.385	39.876
800	154.808	231.616	148.166	66.759	-827.216	-492.393	32.150
900	160.247	250.172	158.484	82.519	-825.055	-450.671	26.156
1000	164.850	267.303	168.520	98.783	-823.237	-409.177	21.373
1100	168.406	283.188	178.231	115.452	-822.032	-367.813	17.466
1200	171.126	297.962	187.601	132.434	-820.081	-326.624	14.218
1300	173.218	311.747	196.626	149.657	-816.357	-285.654	11.478
1400	174.682	324.640	205.315	167.055	-812.653	-244.970	9.140
1500	175.728	336.729	213.677	184.579	-809.013	-204.549	7.123

Iron Iodide (FeI2) — CRYSTAL — $M_r = 309.6560$

Fe I$_2$(cr)

$S°(298.15\ K) = [167.360 \pm 8.4]\ J·K^{-1}·mol^{-1}$
$T_{trs}H° = 650\ K$
$T_{fus}H° = 860 \pm 2\ K$

$\Delta_f H°(0\ K) = $ Unknown
$\Delta_f H°(298.15\ K) = -104.60 \pm 8.4\ kJ·mol^{-1}$
$\Delta_{trs}H° = 0.8\ kJ·mol^{-1}$
$\Delta_{fus}H° = [44.769]\ kJ·mol^{-1}$

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

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	
0							
100							
200							
298.15	83.680	167.360	167.360	0.	-104.600	-111.725	19.574
300	83.680	167.878	167.362	0.155	-104.592	-111.769	19.461
400	83.931	191.983	170.647	8.535	-120.478	-113.639	14.840
500	84.182	210.741	176.859	16.941	-163.121	-107.843	11.266
600	84.425	226.111	183.825	25.371	-161.531	-96.941	8.439
						I <---> II TRANSITION	
650.000	84.546	232.873	187.341	29.596	-158.983		
650.000	87.864	234.160	187.341	30.432	-156.060	-86.362	6.444
700	95.395	240.947	190.927	35.013		-76.173	4.974
800	110.876	254.699	198.037	45.330			
						II <---> LIQUID	
860.000	120.005	263.045	202.281	52.257			
900	126.224	268.644	205.106	57.184	-152.024	-66.419	3.855
1000	136.817	282.555	212.158	70.397	-147.361	-57.157	2.986
1100	141.188	295.834	219.168	84.333	-142.883	-48.336	2.295
1200	142.256	308.176	226.078	98.517	-137.621	-39.991	1.741
1300	142.256	319.562	232.837	112.743	-130.695	-32.137	1.291
1400	142.256	330.105	239.413	126.969	-123.883	-24.812	0.926
1500	142.256	339.919	245.790	141.194	-117.196	-17.970	0.626

Enthalpy of Formation

The chemical equilibrium of the decomposition of FeI$_2$(cr), 771.15–858.15 K, has been studied by Zaugg and Gregory.[1] Using the reported partial pressures for I$_2$(g), the enthalpy change, $\Delta_r H°$(298.15 K), for the reaction FeI$_2$(cr) = Fe(cr) + I$_2$(g) was evaluated by both the 2nd and 3rd law methods to be 39.79 ± 1.0 and 39.69 ± 0.3 kcal·mol⁻¹, respectively. Based on the 3rd law $\Delta_r H°$(298.15 K) value, the enthalpy of formation, $\Delta_f H°$(298.15 K) for FeI$_2$(cr) was calculated as -25 kcal·mol⁻¹ which was adopted here.

The enthalpy change for the reaction FeI$_2$(cr) = Fe⁺⁺(aq) + 2 I⁻(aq) was determined to be -19.46 ± 0.03 kcal·mol⁻¹ by Paoletti et al.[2] using a solution calorimetric method. Adopting $\Delta_f H°$(298.15 K) = -21.3 and -13.19 kcal·mol⁻¹ for Fe⁺⁺(aq) and I⁻(aq), respectively, the value of $\Delta_f H°$(FeI$_2$, cr, 298.15 K) was derived as -28.22 ± 1 kcal·mol⁻¹. The value of $\Delta_f H°$(I⁻, aq, 298.15 K) was taken from Wagman et al.[3] The value of $\Delta_f H°$(Fe⁺⁺, aq, 298.15 K) was derived from enthalpy of solution and formation for FeCl$_2$(cr).

The enthalpies of solution of Fe(cr), I$_2$(cr) and FeI$_2$(cr) in aqueous Br$_2$-KBr solution were measured by Hieber and Woerner[4] using an ice calorimeter. From the results obtained the enthalpy of formation for FeI$_2$(cr) was reported as -30.1 kcal·mol⁻¹.

Heat Capacity and Entropy

The heat capacities, 343.15–773.15 K, were measured by Oetting and Gregory.[5] The $C_p°$ value at temperatures below 343.15 and above 773.15 K were estimated by graphic extrapolation. The low temperature heat capacities, 11–130 K were determined by Miljutin and Parfenova.[6] These data appear to be inadequate for the derivation of the entropy at 298.15 K. The value of $S°$(298.15 K) adopted was calculated from the entropy change, $\Delta_{trs}S°$(298.15 K) = 28.7 cal·K⁻¹·mol⁻¹, for the decomposition reaction FeI$_2$(cr) = Fe(cr) + I$_2$(g), obtained by the second law analysis on the equilibrium pressure data reported by Zaugg and Gregory.[1]

Transition Data

A minor transition in the vicinity of 370°C (360–385°C) has been reported by Oetting and Gregory.[5] Subsequent studies by Wydeven[7] have shown the magnitude of the transition to be sensitive to trace amounts of impurities, but the nature of the transition has not been clearly established. A magnetic transition at 10 K was reported by Bizette et al.[8] The $\Delta_{trs}H°$ value was evaluated from the heat capacity-temperature plot given by Oetting and Gregory.[5]

Fusion Data

T_{fus} was reported by Fischer and Gewehr.[9] $\Delta_{fus}H°$ was estimated by comparison with that for FeBr$_2$(cr).

Sublimation Data

$\Delta_{sub}H°$(cr → monomer, 298.15 K) is calculated as the difference between $\Delta_f H°$(298.15 K) for FeI$_2$(g) and FeI$_2$(cr). $\Delta_{sub}H°$(cr → dimer, 298.15 K) was calculated as the difference between those for Fe$_2$I$_4$(g) and 2 FeI$_2$(cr).

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CURRENT: September 1966

Iron Iodide (FeI₂) LIQUID $M_r = 309.6560$ Iron Iodide (FeI₂) FeI₂(l)

$S°(298.15\ K) = [195.430]\ J\cdot K^{-1}\cdot mol^{-1}$

$T_{fus} = 860 \pm 2\ K$

$\Delta_f H°(298.15\ K) = [-71.046]\ kJ\cdot mol^{-1}$

$\Delta_{fus} H° = 44.769\ kJ\cdot mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(FeI_2, l, 298.15\ K)$ is calculated from $\Delta_f H°(FeI_2, cr, 298.15\ K)$ by adding the enthalpy of fusion, $\Delta_{fus} H°$, and the difference in enthalpy, $H°(860\ K) - H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The heat capacity is assumed to be constant in the temperature range from 298.15 to 2000 K and is calculated on the assumption that $C_p° = 9.0\ cal\cdot K^{-1}\cdot g\text{-atom}^{-1}$ for FeI₂(l). $S°(FeI_2, l, 298.15\ K)$ is calculated in a manner analogous to that used for the enthalpy of formation.

Vaporization Data

T_{vap} is the temperature at which the vapor pressure of FeI₂(g) and Fe₂I₄(g) over FeI₂(l) equals one bar The value of $\Delta_{vap} H°$ is derived from the vapor composition and the enthalpies of vaporization of FeI₂(l) to monomer and dimer at T_{vap}.

T/K	Cp°	S°	-(G°-H°(Tr))/T	H°-H°(Tr)	ΔfH°	ΔfG°	log Kf
	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
0							
100							
200							
298.15	112.968	195.430	195.430	0.	-71.046	-86.540	15.161
300	112.968	196.129	195.433	0.209	-70.984	-86.636	15.085
400	112.968	228.628	199.864	11.506	-83.953	-91.771	11.984
500	112.968	253.836	208.231	22.803	-123.705	-89.975	9.400
600	112.968	274.433	217.600	34.099	-119.249	-83.652	7.283
700	112.968	291.847	226.995	45.396	-115.045	-78.055	5.825
800	112.968	306.931	236.065	56.693	-111.142	-73.041	4.769
860.000	112.968	315.101	241.298	63.471	II <---> LIQUID	---	---
900	112.968	320.237	244.693	67.990	-107.664	-68.493	3.975
1000	112.968	332.140	252.853	79.287	-104.917	-64.297	3.359
1100	112.968	342.907	260.558	90.583	-103.078	-60.310	2.864
1200	112.968	352.736	267.836	101.880	-100.704	-56.546	2.461
1300	112.968	361.778	274.719	113.177	-96.706	-53.029	2.131
1400	112.968	370.150	281.240	124.474	-92.823	-49.816	1.859
1500	112.968	377.944	287.430	135.771	-89.065	-46.876	1.632
1600	112.968	385.235	293.318	147.067	-85.440	-44.183	1.442
1700	112.968	392.084	298.928	158.364	-82.907	-41.693	1.281
1800	112.968	398.541	304.285	169.661	-79.907	-39.356	1.142
1900	112.968	404.649	309.408	180.958	-91.159	-36.479	1.003
2000	112.968	410.443	314.316	192.255	-88.705	-33.665	0.879

Standard State Pressure = $p° = 0.1\ MPa$

Enthalpy Reference Temperature = $T_r = 298.15\ K$

Iron Iodide (FeI₂)

CRYSTAL(I-II)-LIQUID

$M_r = 309.6560$

0 to 650 K crystal, I
650 to 860 K crystal, II
above 860 K liquid

Refer to the individual tables for details.

Iron Iodide (FeI₂)   FeI₂(cr,l)

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹·mol⁻¹				kJ·mol⁻¹		
0	0						
100							
200							
298.15	83.680	167.360	167.360	0.	-104.600	-111.725	19.574
300	83.680	167.878	167.362	0.155	-104.592	-111.769	19.461
400	83.931	191.985	170.647	8.535	-120.478	-113.639	14.840
500	84.182	210.741	176.859	16.941	-163.121	-107.843	11.266
600	84.425	226.111	183.825	25.371	-161.531	-96.941	8.439
650.000	84.546	232.873	187.341	29.596			
650.000	87.864	234.160	187.341	30.432			
			I <--> II TRANSITION				
700	95.395	240.947	190.927	35.013	-158.983	-86.362	6.444
800	110.876	254.699	198.037	45.330	-156.060	-76.173	4.974
860.000	120.005	263.045	202.281	52.257			
860.000	112.968	315.101	202.281	97.026			
			II <--> LIQUID TRANSITION				
900	112.968	320.237	207.410	101.544	-107.664	-68.493	3.975
1000	112.968	332.140	219.298	112.841	-104.917	-64.297	3.359
1100	112.968	342.907	230.054	124.138	-103.078	-60.310	2.864
1200	112.968	352.736	239.874	135.435	-100.704	-56.546	2.461
1300	112.968	361.778	248.908	146.731	-96.706	-53.029	2.131
1400	112.968	370.150	257.273	158.028	-92.823	-49.816	1.859
1500	112.968	377.944	265.061	169.325	-89.065	-46.876	1.632
1600	112.968	385.235	272.346	180.622	-85.440	-44.183	1.442
1700	112.968	392.084	279.190	191.919	-82.907	-41.693	1.281
1800	112.968	398.541	285.643	203.215	-79.907	-39.356	1.142
1900	112.968	404.648	291.747	214.512	-91.159	-36.479	1.003
2000	112.968	410.443	297.538	225.809	-88.705	-33.665	0.879

Iron Iodide (FeI₂)   FeI₂(cr,l)

Iron Iodide (FeI2) IDEAL GAS $M_r = 309.6560$ Iron Iodide (FeI2) FeI2(g)

$S°(298.15 \text{ K}) = [349.597] \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = [89.40 \pm 12.6] \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = [87.86 \pm 12.6] \text{ kJ·mol}^{-1}$

Standard State Pressure = $p° = 0.1$ MPa

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	-16.167	89.402	89.402	INFINITE
100	53.921	286.148	402.435	-11.629	90.467	68.558	-35.811
200	59.295	325.577	355.125	-5.910	89.485	46.951	-12.262
250	60.288	338.925	350.596	-2.918	88.712	36.404	-7.606
298.15	60.859	349.597	349.597	0.	87.864	26.405	-4.626
300	60.876	349.973	349.598	0.113	87.829	26.024	-4.531
350	61.248	359.387	350.341	3.166	86.783	15.802	-2.358
400	61.498	367.583	351.995	6.235	69.686	6.286	-0.821
450	61.675	374.838	354.138	9.315	67.335	-1.499	0.174
500	61.806	381.343	356.538	12.402	24.804	-5.219	0.545
600	62.003	392.630	361.641	18.593	24.154	-11.167	0.972
700	62.180	402.200	366.769	24.802	23.270	-16.987	1.268
800	62.388	410.517	371.729	31.030	22.104	-22.663	1.480
900	62.645	417.879	376.455	37.281	20.537	-28.169	1.635
1000	62.955	424.495	380.934	43.561	18.267	-33.469	1.748
1100	63.308	430.512	385.172	49.874	15.122	-38.476	1.827
1200	63.690	436.036	389.183	56.224	12.549	-43.254	1.883
1300	64.085	441.150	392.987	62.612	11.639	-47.868	1.923
1400	64.479	445.914	396.599	69.041	10.653	-52.409	1.955
1500	64.861	450.375	400.037	75.508	9.582	-56.876	1.981
1600	65.220	454.573	403.315	82.012	8.414	-61.269	2.000
1700	65.551	458.537	406.448	88.551	6.189	-65.567	2.015
1800	65.850	462.292	409.447	95.121	4.462	-69.739	2.024
1900	66.121	465.860	412.323	101.720	-11.487	-73.109	2.010
2000	66.340	469.257	415.086	108.343	-13.707	-76.295	1.993
2100	66.533	472.499	417.743	114.987	-15.974	-79.369	1.974
2200	66.691	475.597	420.303	121.648	-18.285	-82.334	1.955
2300	66.818	478.565	422.772	128.324	-20.637	-85.193	1.935
2400	66.916	481.411	425.156	135.011	-23.023	-87.949	1.914
2500	66.987	484.144	427.462	141.706	-25.434	-90.605	1.893
2600	67.034	486.772	429.693	148.407	-27.861	-93.163	1.872
2700	67.059	489.303	431.854	155.112	-30.296	-95.629	1.850
2800	67.065	491.742	433.949	161.819	-32.728	-98.004	1.828
2900	67.051	494.095	435.983	168.525	-35.148	-100.293	1.806
3000	67.031	496.368	437.958	175.229	-37.549	-102.498	1.785
3100	66.994	498.565	439.878	181.930	-39.924	-104.624	1.763
3200	66.947	500.691	441.745	188.628	-390.566	-99.249	1.620
3300	66.892	502.751	443.563	195.320	-391.362	-90.140	1.427
3400	66.829	504.747	445.333	202.006	-391.743	-81.018	1.245
3500	66.760	506.683	447.059	208.683	-392.110	-71.884	1.073
3600	66.686	508.563	448.741	215.358	-392.462	-62.740	0.910
3700	66.609	510.389	450.383	222.022	-392.799	-53.586	0.756
3800	66.529	512.164	451.985	228.679	-393.121	-44.423	0.611
3900	66.447	513.891	453.551	235.328	-393.430	-35.251	0.472
4000	66.363	515.572	455.080	241.969	-393.726	-26.071	0.340
4100	66.278	517.210	456.576	248.601	-394.012	-16.883	0.215
4200	66.193	518.806	458.038	255.224	-394.289	-7.688	0.096
4300	66.108	520.363	459.470	261.839	-394.560	1.513	-0.018
4400	66.024	521.881	460.871	268.446	-394.827	10.721	-0.127
4500	65.940	523.364	462.243	275.044	-395.093	19.935	-0.231
4600	65.857	524.813	463.588	281.634	-395.360	29.155	-0.331
4700	65.776	526.228	464.906	288.216	-395.631	38.380	-0.477
4800	65.695	527.612	466.198	294.789	-395.908	47.612	-0.518
4900	65.616	528.966	467.465	301.355	-396.195	56.849	-0.606
5000	65.539	530.291	468.708	307.912	-396.495	66.092	-0.690
5100	65.463	531.588	469.928	314.463	-396.809	75.341	-0.772
5200	65.389	532.858	471.126	321.005	-397.142	84.596	-0.850
5300	65.316	534.103	472.303	327.540	-397.497	93.856	-0.925
5400	65.246	535.323	473.459	334.068	-397.612	103.124	-0.998
5500	65.177	536.520	474.594	340.589	-397.875	112.398	-1.067
5600	65.109	537.694	475.711	347.104	-398.282	121.679	-1.135
5700	65.044	538.845	476.808	353.611	-398.719	130.968	-1.200
5800	64.980	539.976	477.888	360.111	-399.192	140.265	-1.263
5900	64.918	541.086	478.950	366.607	-399.702	149.570	-1.324
6000	64.858	542.177	479.994	373.096	-400.254	158.884	-1.383

CURRENT: September 1966 (1 bar)

Electronic Levels and Quantum Weights

ϵ_i, cm⁻¹	g_i
0	[10]
[4200]	[10]
[6800]	[5]

Vibrational Frequencies and Degeneracies

ν_i, cm⁻¹

[140] (1)
[32] (2)
[280] (1)

$\sigma = 2$

Point Group: [D∞h]
Bond Distance: Fe-I = [2.43] Å
Bond Angle: I-Fe-I = [180]°
Rotational Constant $B_0 = [0.011248]$ cm⁻¹

Enthalpy of Formation

The chemical equilibria for the reactions. (A) FeI2(cr) = FeI2(g), (B) FeI2(l) = FeI2(g), and (C) Fe(cr) + 2 I(g) = FeI2(g), have been studied by several investigators. Based on the equilibrium pressures reported, the corresponding enthalpy changes were evaluated by both the 2nd and 3rd law method. The results obtained are presented in the table below. Using the third law $\Delta_f H°(298.15 \text{ K})$ values, the enthalpy of formation for FeI2(g) were calculated. The adopted value for $\Delta_f H°(298.15 \text{ K})$ is 21.0 ± 3 kcal·mol⁻¹. The disagreement between the sets of 2nd and 3rd law $\Delta_f H°(298.15 \text{ K})$ values listed in the table may be due to the presence of dimer, Fe2I4(g) which was not accounted for in deriving the partial pressure of FeI2(g). The data obtained from Schoonmaker et al. was corrected for the presence of dimer. However, only one point value was given.

Source	Reaction	T/K	Method	$\Delta_f H°(298.15 \text{ K})$, kcal·mol⁻¹ 2nd law	3rd law	Drift cal·K⁻¹·mol⁻¹	$\Delta_f H°(298.15 \text{ K})$ kcal·mol⁻¹
Schafer and Honest[1]	A	790.15-850.15	Transpiration	41.81	45.58	+5.78	21.58
	B	874.15-959.15	Transpiration	43.56	35.58	-8.75	18.6
Schoonmaker et al.[2]	A	714	Mass Spectrometric	-	46.78	-	21.78
Sime and Gregory[3]	A	670.0-740.0	Torsion-Effusion	45.13	45.70	0.85	20.7
Zugg and Gregory[4]	C	865.15-1023.15	Transpiration	-32.53	-28.99	3.75	22.1

*The vapor pressure data used for evaluation were those corrected by Zugg and Gregory.[4]

Heat Capacity and Entropy

The molecular structure was assumed to be linear. The Fe-I bond distance was estimated so that the derived Gibbs energy fucntions yielded 2nd and 3rd law $\Delta_f H°(298.15 \text{ K})$ values in reasonable agreements, see the above table. The electronic levels and quantum weights were estimated from those for FeCl2(g) reported by DeKock and Gruen.[6] The vibrational frequencies were estimated by Brewer et al.[5] The vibrational frequencies were in reasonable agreements.

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[6] C. W. DeKock and D. M. Gruen, J. Chem. Phys. 44, 4387 (1966).

PREVIOUS September 1966 (1 atm) Iron Iodide (FeI2)

Iron Oxide (FeO)   CRYSTAL $M_r = 71.8464$ Fe₃O₁(cr)

$S°(298.15\ K) = [60\ 752]$ J K⁻¹·mol⁻¹
$T_{fus} = [1650]$ K

$\Delta_f H°(0\ K) =$ Unknown
$\Delta_f H°(298.15\ K) = [-272.044]$ kJ·mol⁻¹
$\Delta_{fus} H° = [24\ 058]$ kJ·mol⁻¹

Enthalpy of Formation

The value of $\Delta_f H°(298.15\ K)$ for FeO(cr) was derived based on an assumption that at 1650 K, $\Delta_f F°(FeO, cr) = \Delta_f F°(FeO, l)$. From the value $\Delta_f F°(FeO, cr, 1650\ K) = -39.77$ kcal mol⁻¹, $\Delta_f H°(FeO, cr, 1650\ K)$ was calculated to be -63.97 kcal mol⁻¹, yielding $\Delta_f H°(FeO, cr, 298.15\ K) = -65.02$ kcal mol⁻¹ (-272.044 kJ·mol⁻¹).

Heat Capacity and Entropy

The $C_p°$ values were estimated assuming $C_p°(FeO, cr) = C_p°(Wustite, cr) + 0.053\ C_p°(Fe, cr)$. The $C_p°$ values obtained were plotted. The adopted $C_p°$ points were taken from the smoothed $C_p°$ curve $S°(298.15\ K)$ for FeO(cr) was calculated as $S°(FeO, cr) = S°$ (Wustite, cr) + 0 053 $S°(Fe, cr) + \Delta S°(mixing)$ where $\Delta S°(mixing)$ is the entropy of mixing (0.41 cal K⁻¹·mol⁻¹).

Fusion Data

T_{fus} is assumed to be the same as that for Wustite. The difference between $\Delta_f H°(1650\ K)$ for FeO(l) and FeO(cr) is $\Delta_{fus} H°$.

Sublimation Data

$\Delta_{sub} H°(298.15\ K)$ is calculated as the difference between $\Delta_f H°(298\ 15\ K)$ for FeO(g) and FeO(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					
100							
200							
298.15	49.915	60.752	60.752	0.	-272.044	-251.429	44.049
300	49.999	61.061	60.753	0.092	-272.025	-251.301	43.755
400	51.840	75.704	62.737	5.187	-271.044	-244.543	31.934
500	53.388	87.438	66.541	10.449	-270.164	-238.022	24.866
600	54.894	97.309	70.868	15.865	-269.414	-231.666	20.168
700	56.149	105.856	75.270	21.418	-268.814	-225.425	16.821
800	57.321	113.443	79.577	27.093	-268.422	-219.256	14.316
900	58.283	120.249	83.724	32.872	-268.374	-213.118	12.369
1000	59.371	126.447	87.691	38.756	-268.969	-206.955	10.810
1100	60.234	132.146	91.477	44.736	-270.385	-200.670	9.529
1200	61.086	137.424	95.089	50.802	-271.184	-194.316	8.458
1300	61.975	142.349	98.537	56.956	-270.265	-187.947	7.552
1400	62.760	146.971	101.833	63.194	-269.361	-181.649	6.777
1500	63.396	151.323	104.989	69.502	-268.484	-175.415	6.108
1600	64.015	155.435	108.014	75.873	-267.642	-169.238	5.525
1650.000	64.319	157.409	109.481	79.081	CRYSTAL <---> LIQUID	---	---
1700	64.651	159.334	110.919	82.305	-267.784	-163.094	5.011
1800	65.229	163.045	113.713	88.798	-267.345	-156.949	4.555
1900	65.790	166.587	116.403	95.349	-281.041	-150.125	4.127
2000	66.316	169.975	118.998	101.955	-280.919	-143.237	3.741

PREVIOUS: CURRENT. June 1965

Iron Oxide (FeO)   Fe₃O₁(cr)

Iron Oxide (FeO) LIQUID $M_r = 71.8464$ Iron Oxide (FeO) Fe₁O₁(l)

$S°(298.15\ K) = 75.415\ \mathrm{J\cdot K^{-1}\cdot mol^{-1}}$
$\Delta_f H°(298.15\ K) = [-249.532]\ \mathrm{kJ\cdot mol^{-1}}$
$T_{fus} = [1650]\ K$
$\Delta_{fus}H° = [24\ 058]\ \mathrm{kJ\cdot mol^{-1}}$

Enthalpy of Formation

The enthalpy of formation, $\Delta_f H°(\mathrm{FeO}, l, 298.15\ K)$, is evaluated based on as assumption that the enthalpy of fusion of $O_2(g)$. In other words, during melting the Wustite releases $O_2(g)$ and converts tp FeO(l).

Heat Capacity and Entropy

The enthalpy changes, $H°(T)-H°(298.15\ K)$, for 1650–1800 K of liquid iron oxide were determined by Coughlin et al.[1] The $C_p°(\mathrm{FeO}, l)$ was derived as 16.3 cal·K⁻¹. This value was adopted as the heat capacity for FeO(l) up to 4000 K. A glass transition temperature was assumed at 1100 K. $S°(\mathrm{FeO}, l, 298.15\ K)$ is calculated based on an assumption that the entropy of fusion of Wustite represents also the entropy change of the reaction. $\mathrm{Fe_{0.947}O(cr)} = 0.947\ \mathrm{FeO(l)} + (0.053/2)\ O_2(g)$. From the entropy of fusion, $\Delta_{fus}H°(1650\ K) = 4.539\ \mathrm{cal\cdot K^{-1}\cdot mol^{-1}}$, the value $S°(\mathrm{FeO}), l, 298.15\ K) = 18.029\ \mathrm{cal\cdot K^{-1}\cdot mol^{-1}}$ was derived.

Fusion Data

The melting point (T_{fus}) for Wustite ($\mathrm{Fe_{0.947}O}$, cr) has been reported by many investigators. However, the composition of the liquid state of Wustite was not identified. An assumption was made that during melting the reaction $\mathrm{Fe_{0.947}O(cr)} = 0.947\ \mathrm{FeO(l)} + (0.053/2)\ O_2(cr)$ occurs. Hence the related thermodynamic properties were derived.

Decomposition Data

T_{des} is the temperature at which $\Delta_f G°$ equals zero.

Reference

1. J. P. Coughlin, E. G. King and K. R. Bonnickson, J. Amer. Chem. Soc. **73**, 3891 (1951).

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

T/K	C°p	S°	-(G°-H°(Tr))/T	H°-H°(Tr)	ΔfH°	ΔfG°	log Kf
		J·K⁻¹·mol⁻¹			kJ·mol⁻¹		
0							
100							
200							
298.15	48.116	75.415	75.415	0.	-249.532	-233.289	40.871
300	48.183	75.713	75.416	0.089	-249.517	-233.189	40.602
400	50.380	89.893	77.334	5.023	-248.696	-227.871	29.757
500	51.848	101.298	81.023	10.137	-247.965	-222.752	23.271
600	53.028	110.857	85.220	15.382	-247.385	-217.766	18.958
700	54.070	119.110	89.485	20.737	-246.983	-212.864	15.884
800	55.041	126.394	93.653	26.193	-246.810	-208.005	13.581
900	55.969	132.931	97.660	31.744	-246.991	-203.148	11.790
1000	56.873	138.875	101.489	37.386	-247.827	-198.241	10.355
1100	57.761	144.337	105.139	43.118	-249.492	-193.187	9.174
1100.000	57.761	144.337	105.139	43.118	-249.537	GLASS <--> LIQUID	
1100.000	68.199	144.337	105.139	43.118		TRANSITION	
1200	68.199	150.271	108.656	49.938	-247.952	-188.086	8.187
1300	68.199	155.730	112.070	56.758	-246.466	-183.030	7.354
1400	68.199	160.784	115.371	63.578	-245.077	-178.092	6.645
1500	68.199	165.490	118.558	70.398	-243.785	-173.257	6.033
1600	68.199	169.891	121.630	77.218		-168.512	5.501
1650.000	68.199	171.990	123.124	80.628	-243.785	CRYSTAL <--> LIQUID	
1700	68.199	174.026	124.592	84.038	-243.540	-163.826	5.034
1800	68.199	177.924	127.447	90.858	-242.774	-159.160	4.619
1900	68.199	181.611	130.202	97.678	-256.202	-153.831	4.229
2000	68.199	185.109	132.861	104.497	-255.866	-148.452	3.877
2100	68.199	188.437	135.428	111.317	-255.541	-143.089	3.559
2200	68.199	191.609	137.911	118.137	-255.227	-137.741	3.270
2300	68.199	194.641	140.312	124.957	-254.925	-132.408	3.007
2400	68.199	197.543	142.636	131.777	-254.634	-127.088	2.766
2500	68.199	200.327	144.889	138.597	-254.354	-121.779	2.544
2600	68.199	203.002	147.073	145.417	-254.085	-116.481	2.340
2700	68.199	205.576	149.192	152.237	-253.826	-111.194	2.151
2800	68.199	208.056	151.250	159.057	-253.577	-105.915	1.976
2900	68.199	210.450	153.251	165.877	-253.338	-100.646	1.813
3000	68.199	212.762	155.196	172.697	-253.109	-95.385	1.661
3100	68.199	214.998	157.089	179.517	-252.890	-90.131	1.519
3200	68.199	217.163	158.933	186.336	-600.979	-77.460	1.264
3300	68.199	219.262	160.729	193.156	-598.876	-61.133	0.968
3400	68.199	221.298	162.481	199.976	-596.815	-44.869	0.689
3500	68.199	223.275	164.190	206.796	-594.795	-28.665	0.428
3600	68.199	225.196	165.858	213.616	-592.816	-12.518	0.182
3700	68.199	227.064	167.487	220.436	-590.880	3.575	-0.050
3800	68.199	228.883	169.079	227.256	-588.987	19.616	-0.270
3900	68.199	230.655	170.635	234.076	-587.137	35.608	-0.477
4000	68.199	232.381	172.157	240.896	-585.331	51.553	-0.673
4100	68.199	234.065	173.647	247.716	-583.570	67.453	-0.859
4200	68.199	235.709	175.105	254.536	-581.855	83.311	-1.036
4300	68.199	237.314	176.533	261.356	-580.186	99.128	-1.204
4400	68.199	238.881	177.932	268.176	-578.566	114.907	-1.364
4500	68.199	240.414	179.304	274.995	-576.993	130.650	-1.517
4600	68.199	241.913	180.649	281.815	-575.470	146.158	-1.662
4700	68.199	243.380	181.968	288.635	-573.998	162.034	-1.801
4800	68.199	244.816	183.262	295.455	-572.578	177.680	-1.934
4900	68.199	246.222	184.533	302.275	-571.212	193.296	-2.061
5000	68.199	247.600	185.781	309.095	-569.900	208.885	-2.182

Iron Oxide (FeO)   Fe₁O₁(l)

Iron Oxide (FeO) $M_r = 71.8464$ Fe₁O₁(cr,l)

CRYSTAL-LIQUID

0 to 1650 K crystal
above 1650 K liquid

Refer to the individual tables for details.

Iron Oxide (FeO)

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

T/K	$C°_p$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
0							
100							
200							
298.15	49.915	60.752	60.752	0.	-272.044	-251.429	44.049
300	49.999	61.061	60.753	0.092	-272.025	-251.301	43.755
400	51.840	75.704	62.737	5.187	-271.044	-244.543	31.934
500	53.388	87.438	66.541	10.449	-270.164	-238.022	24.866
600	54.894	97.309	70.868	15.865	-269.414	-231.666	20.168
700	56.149	105.866	75.270	21.418	-268.814	-225.425	16.821
800	57.321	113.443	79.577	27.093	-268.422	-219.256	14.316
900	58.283	120.249	83.724	32.872	-268.374	-213.118	12.369
1000	59.371	126.447	87.691	38.756	-268.969	-206.955	10.810
1100	60.234	132.146	91.477	44.736	-270.385	-200.670	9.529
1200	61.086	137.424	95.089	50.802	-271.184	-194.316	8.458
1300	61.975	142.349	98.537	56.956	-270.265	-187.947	7.552
1400	62.760	146.971	101.833	63.194	-269.361	-181.649	6.777
1500	63.396	151.323	104.989	69.502	-268.484	-175.415	6.108
1600	64.015	155.435	108.014	75.873	-267.642	-169.238	5.525
1650.000	64.319	157.409	109.481	79.081			—
CRYSTAL <--> LIQUID TRANSITION							
1650.000	68.199	171.990	109.481	103.139	-243.540	-163.826	5.034
1700	68.199	174.026	111.350	106.549	-242.774	-159.160	4.619
1800	68.199	177.924	114.941	113.369	-256.202	-153.831	4.229
1900	68.199	181.611	118.354	120.189	-255.866	-148.452	3.877
2000	68.199	185.109	121.605	127.009	-255.541	-143.089	3.559
2100	68.199	188.437	124.709	133.829	-255.227	-137.741	3.270
2200	68.199	191.609	127.678	140.649	-254.925	-132.408	3.007
2300	68.199	194.641	130.524	147.468	-254.634	-127.088	2.766
2400	68.199	197.543	133.257	154.288	-254.354	-121.779	2.544
2500	68.199	200.327	135.884	161.108	-254.085	-116.481	2.340
2600	68.199	203.002	138.415	167.928	-253.826	-111.194	2.151
2700	68.199	205.576	140.855	174.748	-253.577	-105.915	1.976
2800	68.199	208.056	143.211	181.568	-253.338	-100.646	1.813
2900	68.199	210.450	145.488	188.388	-253.109	-95.385	1.661
3000	68.199	212.762	147.692	195.208	-252.890	-90.131	1.519
3100	68.199	214.998	149.828	202.028			
3200	68.199	217.163	151.898	208.848	-600.979	-77.460	1.264
3300	68.199	219.262	153.908	215.668	-598.876	-61.133	0.968
3400	68.199	221.298	155.860	222.488	-596.815	-44.869	0.689
3500	68.199	223.275	157.758	229.308	-594.795	-28.665	0.428
3600	68.199	225.196	159.605	236.127	-592.816	-12.518	0.182
3700	68.199	227.064	161.403	242.947	-590.880	3.575	-0.050
3800	68.199	228.883	163.155	249.767	-588.987	19.616	-0.270
3900	68.199	230.655	164.863	256.587	-587.137	35.608	-0.477
4000	68.199	232.381	166.530	263.407	-585.331	51.552	-0.673
4100	68.199	234.065	168.156	270.227	-583.570	67.453	-0.859
4200	68.199	235.709	169.745	277.047	-581.855	83.310	-1.036
4300	68.199	237.314	171.298	283.867	-580.186	99.128	-1.204
4400	68.199	238.881	172.816	290.687	-578.566	114.907	-1.364
4500	68.199	240.414	174.301	297.507	-576.993	130.650	-1.517
4600	68.199	241.913	175.755	304.327	-575.470	146.358	-1.662
4700	68.199	243.380	177.178	311.147	-573.998	162.034	-1.801
4800	68.199	244.816	178.573	317.966	-572.578	177.679	-1.934
4900	68.199	246.222	179.939	324.786	-571.212	193.296	-2.061
5000	68.199	247.600	181.278	331.606	-569.900	208.883	-2.182

Iron Oxide (FeO) Fe₁O₁(cr,l)

Iron Oxide (FeO)   IDEAL GAS   Fe₁O₁(g)

$M_r = 71.8464$ Iron Oxide (FeO)

Fe₁O₁(g)   Standard State Pressure = $p° = 0.1$ MPa

$S°(298.15\ \mathrm{K}) = [241.924]\ \mathrm{J \cdot K^{-1} \cdot mol^{-1}}$

$\Delta_f H°(0\ \mathrm{K}) = 251.05 \pm 20.9\ \mathrm{kJ \cdot mol^{-1}}$
$\Delta_f H°(298.15\ \mathrm{K}) = 251.04 \pm 20.9\ \mathrm{kJ \cdot mol^{-1}}$

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	$\log K_f$
	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	
0	0.	0.	INFINITE	-8.837	251.051	251.051	INFINITE
100	29.110	209.460	268.743	-5.928	252.085	240.411	-125.578
200	29.741	229.752	244.739	-2.997	251.791	228.779	-59.751
250	30.538	236.471	242.436	-1.491	251.431	223.067	-46.607
298.15	31.406	241.924	241.924	0.	251.040	217.639	-38.129
300	31.439	242.118	241.924	0.058	251.024	217.431	-37.858
350	32.302	247.030	242.310	1.652	250.594	211.866	-31.619
400	33.065	251.394	243.178	3.287	250.139	206.364	-26.948
450	33.715	255.328	244.313	4.957	249.653	200.921	-23.322
500	34.261	258.909	245.596	6.656	249.127	195.534	-20.427
600	35.098	265.234	248.356	10.127	247.932	184.925	-16.099
700	35.689	270.691	251.166	13.668	245.520	174.532	-13.024
800	36.118	275.486	253.912	17.259	244.828	164.360	-10.732
900	36.439	279.760	256.551	20.888	242.725	154.422	-8.962
1000	36.687	283.612	259.068	24.545	239.904	144.752	-7.561
1100	36.884	287.119	261.461	28.223	236.186	135.431	-6.431
1200	37.048	290.335	263.735	31.920	233.018	126.392	-5.502
1300	37.188	293.306	265.897	35.632	231.495	117.568	-4.724
1400	37.315	296.067	267.954	39.357	229.886	108.864	-4.062
1500	37.434	298.645	269.915	43.095	228.192	100.278	-3.492
1600	37.550	301.065	271.787	46.844	226.413	91.808	-2.997
1700	37.669	303.345	273.577	50.605	223.600	83.471	-2.565
1800	37.792	305.502	275.291	54.378	221.319	75.293	-2.185
1900	37.922	307.548	276.936	58.164	204.857	67.947	-1.868
2000	38.060	309.497	278.516	61.963	202.172	60.811	-1.588
2100	38.207	311.357	280.035	65.776	199.490	53.809	-1.338
2200	38.363	313.138	281.500	69.605	196.812	46.934	-1.114
2300	38.527	314.847	282.913	73.449	194.139	40.182	-0.913
2400	38.699	316.491	284.278	77.310	191.471	33.545	-0.730
2500	38.877	318.074	285.598	81.189	188.810	27.019	-0.565
2600	39.063	319.602	286.877	85.086	186.157	20.600	-0.414
2700	39.253	321.080	288.117	89.002	183.511	14.283	-0.276
2800	39.447	322.511	289.319	92.936	180.875	8.063	-0.150
2900	39.644	323.899	290.488	96.891	178.248	1.938	-0.035
3000	39.842	325.246	291.624	100.865	175.632	-4.097	0.071
3100	40.041	326.556	292.730	104.893	173.025	-10.045	0.169
3200	40.240	327.830	293.807	108.873	-177.870	-8.485	0.139
3300	40.437	329.071	294.857	112.907	-178.553	-3.182	0.050
3400	40.633	330.281	295.881	116.961	-179.258	2.143	-0.033
3500	40.825	331.462	296.881	121.034	-179.985	7.489	-0.112
3600	41.014	332.615	297.858	125.126	-180.734	12.856	-0.187
3700	41.198	333.741	298.812	129.236	-181.508	18.244	-0.258
3800	41.378	334.842	299.746	133.365	-182.305	23.654	-0.325
3900	41.553	335.919	300.660	137.512	-183.129	29.084	-0.390
4000	41.722	336.973	301.555	141.676	-183.979	34.536	-0.451
4100	41.885	338.006	302.431	145.856	-184.838	40.010	-0.510
4200	42.042	339.017	303.290	150.052	-185.766	45.505	-0.566
4300	42.193	340.008	304.133	154.264	-186.706	51.023	-0.620
4400	42.338	340.980	304.959	158.491	-187.678	56.563	-0.671
4500	42.476	341.933	305.770	162.732	-188.685	62.125	-0.721
4600	42.608	342.868	306.566	166.986	-189.727	67.709	-0.769
4700	42.734	343.785	307.349	171.253	-190.808	73.318	-0.815
4800	42.853	344.686	308.117	175.532	-191.929	78.949	-0.859
4900	42.966	345.571	308.872	179.823	-193.091	84.605	-0.902
5000	43.072	346.440	309.615	184.125	-194.297	90.284	-0.943
5100	43.173	347.294	310.346	188.438	-195.549	95.988	-0.983
5200	43.267	348.133	311.064	192.760	-196.849	101.717	-1.022
5300	43.356	348.958	311.771	197.091	-198.200	107.472	-1.059
5400	43.440	349.770	312.468	201.431	-199.604	113.252	-1.095
5500	43.518	350.567	313.153	205.779	-201.063	119.059	-1.131
5600	43.590	351.352	313.828	210.134	-202.581	124.893	-1.165
5700	43.658	352.124	314.493	214.497	-204.161	130.755	-1.198
5800	43.721	352.884	315.149	218.866	-205.805	136.645	-1.231
5900	43.779	353.632	315.795	223.241	-207.518	142.563	-1.262
6000	43.833	354.368	316.431	227.621	-209.302	148.512	-1.293

Electronic Levels and Quantum Weights

State	ϵ, cm⁻¹	g_i
[⁵Δ]	0	[10]
	[10000]	[10]
	[16000]	[5]

$\omega_e = 880.0\ \mathrm{cm^{-1}}$ $\omega_e x_e = 5.0\ \mathrm{cm^{-1}}$ $\sigma = 1$
$B_e = [0.4184]\ \mathrm{cm^{-1}}$ $\alpha_e = [0.00293]\ \mathrm{cm^{-1}}$ $r_e = [1.8]\ \text{Å}$

Enthalpy of Formation

The enthalpy of formation for FeO(g) is not well established at the present time. The values of $\Delta_f H°$(FeO, g, 298.15 K) derived from the following reactions: (A) FeO(g) = Fe(g) + O(g) , (B) FeO(g) + 1/2 O₂(g), and (C) FeO(l) = FeO(g), are not in agreement. There are three $D°_0$(Fe–O) values reported for reaction (1). The enthalpy change for reaction (2) was evaluated based on the partial pressure data (PFeO/ PFe) = 0.2 at 1600°C, measured by Washburn,[4] using a mass spectrometric method,[6] and PO₂ = 1.66 × 10⁻⁶ atm reported by Darken and Gurry.[7] The enthalpy value for reaction (3) was calculated based on the reported value, $\Delta_{sub} H°$(2785 K) = 96.096 kcal·mol⁻¹ determined by Burtsev et al.[5] The results obtained are presented as follows. The value of $\Delta_f H°$(298.15 K) for FeO(g) adopted is 60 ± 5 kcal·mol⁻¹.

Source	Reaction	Method	$\Delta_f H°$(298.15 K), kcal·mol⁻¹	$\Delta_f H°$(298.15 K) kcal·mol⁻¹
Herzberg[1]	A	Spectroscopic	111.9	47.2
Gaydon[2]	A	Spectroscopic	93.4 ± 23.1	65.7 ± 23.1
Lagerqvist and Huldt[3]	A	Spectroscopic	99 0 ± 11.6	60.1 ± 11.6
Washburn et al.[4]	B	Spectroscopic	99.3 ± 5	59.8 ± 5
Burtsev et al.[5]	C	Transpiration	111.8	52.2

Heat Capacity and Entropy

Since the ground state configuration is mainly that due to Fe⁺⁺ in a ligand field, it was assumed to be the same as that for FeCl₄(g) reported by DeKock and Gruen.[8] The electronic levels and quantum weights were estimated by comparison with those for FeCl₄(g). The values of ω_e and $\omega_e x_e$ were taken from Herzberg.[1] The bond distance was calculated by use of the relationship. $B_e = (2.799076 \times 10^{-39})/I$ where I is the moment of inertia of FeO(g). The value of α_e was derived from ω_e, $\omega_e x_e$ and B_e by the method suggested by Herzberg.[1]

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

Iron Oxide (FeO)   Fe₁O₁(g)

Iron Sulfate (FeSO₄)   CRYSTAL $M_r = 151.9046$ Fe₁O₄S₁(cr)

$S°(298.15\ K) = 120.957 \pm 1.3\ \mathrm{J \cdot K^{-1} \cdot mol^{-1}}$

$\Delta_f H°(0\ K) = -919.33 \pm 8.4\ \mathrm{kJ \cdot mol^{-1}}$
$\Delta_f H°(298.15\ K) = -928\ 85 \pm 8\ 4\ \mathrm{kJ \cdot mol^{-1}}$

	Enthalpy Reference Temperature = T_r = 298.15 K				Standard State Pressure = $p°$ = 0.1 MPa		
	$J \cdot K^{-1} \cdot mol^{-1}$				$kJ \cdot mol^{-1}$		
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	-16.769	-919.331	-919.331	INFINITE
100	44.074	42.771	194.810	-15.204	-924.688	-892.445	466.166
200	78.848	85.016	129.562	-8.909	-927.627	-858.919	224.337
298.15	100.583	120.957	120.957	0.	-928.848	-824.879	144.515
300	101.002	121.580	120.959	0.186	-928.859	-824.234	143.512
400	116.650	152.861	125.118	11.097	-931.115	-789.237	103.064
500	128.909	180.266	133.463	23.401	-931.710	-753.695	78.738
600	138.030	204.613	143.331	36.769	-931.332	-718.113	62.517
700	144.641	226.410	153.670	50.918	-930.365	-682.648	50.940
800	149.411	246.052	164.011	65.633	-929.150	-647.342	42.257
900	152.758	263.849	174.131	80.746	-981.132	-611.106	35.468
1000	155.477	280.088	183.927	96.161	-979.245	-570.101	29.779
1100	157.779	295.017	193.356	111.826	-978.112	-529.226	25.131
1200	159.829	308.835	202.411	127.709	-976.304	-488.516	21.265
1300	161.670	321.702	211.098	143.785	-972.740	-448.012	18.001
1400	163.343	333.744	219.433	160.036	-969.161	-407.782	15.215
1500	164.933	345.069	227.435	176.451	-965.573	-367.809	12.808
1600	166.440	355.762	235.124	193.020	-961.981	-328.076	10.711
1700	167.862	365.895	242.521	209.735	-959.340	-288.548	8.866
1800	169.285	375.530	249.645	226.593	-956.087	-249.184	7.231
1900	170.624	384.719	256.514	243.589	-966.938	-209.298	5.754
2000	171.962	393.505	263.146	260.718	-963.937	-169.499	4.427

Enthalpy of Formation

The enthalpy change for the reaction FeSO₄(cr) = FeSO₄(110 ∞H₂O) was determined to be -14.9 kcal·mol⁻¹ by Forcrand.[1] Using $\Delta_f H°$(298.15 K) = -345.85 kcal·mol⁻¹ for FeSO₄(110 ∞H₂O), the enthalpy of formation (298 15 K) for FeSO₄(cr) was calculated as -221 kcal·mol⁻¹. The value of $\Delta_f H°$(FeSO₄, cr, 298 15 K) was estimated based on $\Delta_r H°$(298 15 K) = 235.9 kcal·mol⁻¹ for FeSO₄(200 ∞H₂O) + H₂SO₄(200 H₂O) = FeSO₄(200 H₂O) measured by Thomsen.[2] See the Fe(OH)₂(cr) table for details. The decomposition pressures of FeSO₄(cr) at different temperatures were investigated by D'Ans[3] and Greulich.[4] Using their reported partial pressures for SO₃(g) and SO₂(g), the enthalpy change for the reaction 2FeSO₄(cr) = Fe₂O₃(cr) + SO₃(g) + SO₂(g) was evaluated by both the 2nd and 3rd law methods. The results obtained are presented in the following table.

Source	T/K	$\Delta_r H°$(298.15 K), kcal·mol⁻¹ 2nd law	3rd law	$\Delta_f H°$(298 15 K) kcal·mol⁻¹
D'Ans[3](1905)	753.15-908.15	83.2 ± 4.6	82.7 ± 1.1	-222.7
Greulich[4](1927)	887.15-971.15	64.8 ± 8.8	80.1 ± 1.4	-221.5
Neumann and Heinke[5](1937)	633.15-862.15	72.4 ± 5.4	75.3 ± 0.5	-219.1

The decomposition pressures assumed for the same reaction have been determined by Neumann and Heinke.[5] From their data the partial pressures for SO₃(g) and SO₂(g) were evaluated. Using the derived SO₃(g) and SO₂(g) partial pressures, the corresponding enthalpy change for the reaction were calculated by both the 2nd and 3rd law methods. The results obtained are also listed in the same table.

The value of $\Delta_f H°$(298.15 K) for FeSO₄(cr) is selected as 222 ± 2 kcal·mol⁻¹.

Heat Capacity and Entropy

The low temperature heat capacities, 50.12 294.9 K, were determined by Moore and Kelley.[6] Based on S°(50.12 K) = 2.10 cal·K⁻¹·mol⁻¹, the value of S°(FeSO₄, cr, 298 15 K) was reported to be 25.71 ± 0.2 cal·K⁻¹·mol⁻¹. Using the Gibbs energy functions for FeSO₄(cr) based on this S°(298.15 K) value, to evaluate the vapor pressure data for Reaction,[1] the 2nd and 3rd law values of $\Delta_r H°$(298.15 K) were derived as 72.36 ± 7.60 and 86.51 ± 1.26 kcal mol⁻¹, respectively. Since the report by Moore and Kelley[6] did not mention the magnetic entropy contribution, an attempt was made to add 3.20 (=Rln5) cal·K⁻¹·mol⁻¹ to S°(FeSO₄, cr, 298.15 K) and reevaluate the decomposition pressure data. The results obtained were better than before, see the paragraph on "Enthalpy of Formation," for details. Therefore the value, S°(298.15 K) = 25.71 ± 3.2 = 28.91 cal·K⁻¹·mol⁻¹ for FeSO₄(cr), was adopted. The heat capacities above 294 9 K were estimated by comparison with those for MnSO₄(cr) The high temperature heat capacities, 870.3-1082.3 K, were determined by Southard and Shomate.[7] The two sets of data were joined smoothly at 298.15 K by use of Shomate-function plot.

Decomposition Data

T_{dcm} = 944 K is the temperature at which the vapor pressure of the gaseous decomposition products equals one atmosphere, which was obtained by graphical interpolation of the decomposition pressure data on FeSO₄(cr), reported by Greulich.[4]

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Iron Sulfide, Trollite (FeS) CRYSTAL $M_r = 87.907$ Iron Sulfide, Trollite (FeS) Fe₅S₁(cr)

$S°(298.15 \text{ K}) = 60.321 \pm 0.04 \text{ J·K}^{-1}\cdot\text{mol}^{-1}$

$T_{trs1} = 411 \pm 3 \text{ K}$
$T_{trs2} = 598 \pm 3 \text{ K}$
$T_{fus} = 1463 \pm 3 \text{ K}$

$\Delta_f H°(0 \text{ K}) = -102.17 \pm 0.8 \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = -101.67 \pm 0.8 \text{ kJ·mol}^{-1}$
$\Delta_{trs1}H° = -1.665 \pm 0.8 \text{ kJ·mol}^{-1}$
$\Delta_{trs2}H° = -0.397 \pm 0.08 \text{ kJ·mol}^{-1}$
$\Delta_{fus}H° = 31.464 \pm 2.1 \text{ kJ·mol}^{-1}$

Standard State Pressure = $p° = 0.1$ MPa

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
		J·K⁻¹·mol⁻¹			kJ·mol⁻¹		
0	0.	0.	INFINITE	-9.413	-102.166	-102.166	INFINITE
100	26.670	17.216	99.528	-8.231	-102.096	-101.959	53.258
200	43.052	41.665	64.714	-4.610	-101.886	-101.901	26.614
298.15	50.517	60.321	60.321	0.	-101.671	-101.953	17.862
300	50.671	60.634	60.322	0.094	-101.666	-101.954	17.752
400	89.203	79.060	62.567	6.597	-102.388	-102.086	13.331
411.000	95.051	81.559	63.042	7.610	ALPHA <--> BETA TRANSITION		
411.000	72.358	85.611	63.042	9.276			
500	72.358	99.794	68.363	15.715	-100.050	-102.492	10.707
598.000	72.358	112.745	74.607	22.807	BETA <--> GAMMA TRANSITION		
598.000	62.083	113.409	74.607	23.204			
600	62.030	113.617	74.736	23.328	-99.108	-103.033	8.970
700	59.808	122.999	80.982	29.412	-99.697	-103.645	7.734
800	58.560	130.893	86.740	35.322	-100.612	-104.151	6.800
900	58.286	137.765	92.036	41.156	-155.064	-103.437	6.003
1000	58.986	143.934	96.922	47.012	-155.812	-97.670	5.102
1100	60.662	149.627	101.457	52.986	-157.351	-91.766	4.358
1200	63.311	155.011	105.697	59.177	-158.138	-85.786	3.734
1300	66.935	160.216	109.692	65.681	-156.980	-79.802	3.206
1400	71.533	165.338	113.484	72.596	-155.509	-73.918	2.758
1463.000	74.930	168.560	115.786	77.208	GAMMA <--> LIQUID		
1500	77.106	170.458	117.111	80.020	-153.630	-68.153	2.373
1600	83.653	175.638	120.607	88.050	-151.243	-62.529	2.041
1700	91.174	180.930	123.999	96.783	-149.200	-57.054	1.753
1800	99.670	186.377	127.312	106.317	-145.839	-51.727	1.501
1900	109.140	192.016	130.568	116.749	-155.774	-45.996	1.262

Enthalpy of Formation

The adopted $\Delta_f H°(298.15 \text{ K})$ is 24.30 ± 0.2 kcal·mol⁻¹ and is based on our 3rd law analysis of gas phase H₂S/H₂ equilibrium data of.[1-7] Additional studies of a similar nature are reported by Mills.[8] The gas phase equilibrium results are favored over calorimetric[8] and emf[9-11] results because of greater certainty in the stoichiometry of the iron sulfide. Of the calorimetric studies[8] only those of Adami and King ($\Delta_f H°(298.15 \text{ K}) = -23.89 \pm 0.41$ kcal·mol⁻¹) and the annealed sample of Ariya et al. ($\Delta_f H°(298.15 \text{ K}) = -24.4$ kcal·mol⁻¹) are in reasonable agreement with the adopted value. Of the emf results, all refer to less than stoichiometric composition Fe₀.₉₅S[10] or to impure sample, 97.58%.[11] $\Delta_f H°(298.15 \text{ K})$ has been shown to vary significantly as a function of stoichiometry[12] which is a result of the variation of $\Delta_f H°$ with composition.[12]

Source	Reaction	Method	Data Points	T/K	$\Delta_f H°(298.15 \text{ K})$, kcal·mol⁻¹ 2nd law	3rd law	Drift cal K⁻¹·mol⁻¹	$\Delta_f H°(298.15 \text{ K})$ kcal·mol⁻¹
Rosenqvist[1]	C	H₂S/H₂	11	773-1257	17.89 ± 0.41	-19.40 ± 0.53	-1.45 ± 0.40	-24.30 ± 0.6
Blaise[2]	C	"	equation	923-1043	-17.87	-19.41 ± 0.14	-1.57	-24.31 ± 0.2
Turkdogan[3]	C	"	3	943-1173	-17.24 ± 0.39	-19.40 ± 0.48	-2.03 ± 0.36	-24.30 ± 0.5
Alcock[4]	B	"	equation	720-1261	-38.30	-39.68 ± 0.56	-1.38	-24.26 ± 0.6
McCabe[5]	B	"	10	1224-1255	-33.76 ± 2.84	-39.70 ± 0.15	4.81 ± 2.3	-24.28 ± 0.2
Sudo[6]	C	"	4	1048-1145	-17.39 ± 2.19	-19.51 ± 0.29	-1.95 ± 2.01	-24.41 ± 0.4
Rau[7]	C	"	9	820-1257	-19.40 ± 0.23	-19.31 ± 0.20	0.09 ± 0.22	-24.15 ± 0.3
Berner[9]	A	emf	1	298.15		-24.08		-24.08
DeRanter[10]	A	H titration	1	298.15				-20.55
DeRanter[10]	A	emf	1	298.15		-20.56		-20.56
Guldin[11]	B	emf	1	973		36.445		-21.02

†Reactions: (A) Fe(cr) + S(cr) → FeS(cr), (B) Fe(cr) + 1/2 S₂(g) → FeS(cr), (C) Fe(cr) + H₂S(g) → FeS(cr) + H₂(g)

Heat Capacity and Entropy

The adopted heat capacities are obtained by merging the $C_p°$ data (7-345 K) of Gronvold et al.[13] and the enthalpy data (356-1488 K) of Coughlin.[14] The data are difficult to merge smoothly because of the proximity of the α β transition at 411 K. Coughlin gives the composition of his sample as FeS₁.₀₂ and this introduces some uncertainty at the higher temperatures.

The value of $S°(298.15 \text{ K})$ is obtained from the appropriate integration of $C_p°$ values assuming $S°(7 \text{ K}) = 0.0028$ cal·K⁻¹·mol⁻¹.

Phase Data

The mineral pyrrhotite has a composition range extending from FeS to Fe₀.₈₇₅S (Fe₇S₈). the name troilite is reserved for the stoichiometric FeS composition. The phase diagram[15] of this system shows that the iron rich limit of this phase corresponds to stoichiometric FeS below 1370 K; above this temperature only an iron deficient material exists so that stoichiometric FeS will melt incongruently.

There are two solid state phase transitions, both associated with electronic magnetic phenomena. The adopted temperature of the α β transition is $T_{trs1} = 411 \pm 3$ K.[15] Our analysis of the adopted $C_p°$ data yields $\Delta_{trs1}H° = -0.398$ kcal·mol⁻¹; in view of the uncertainties in these data we adopt an uncertainty of ±0.2 kcal·mol⁻¹ in $\Delta_{trs1}H°$. The adopted temperature of the β-γ transition is $T_{trs2} = 598 \pm 3$ K[15] and our analysis of Coughlin's high temperature enthalpy data[14] yields $\Delta_{trs2}H° = 0.095 \pm 0.02$ kcal·mol⁻¹.

Fusion Data

Refer to the liquid table for details.

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PREVIOUS:

Continued on page 1251

Iron Sulfide, Trollite (FeS) Fe₅S₁(cr)

Iron Sulfide (FeS)   LIQUID $M_r = 87.907$ Fe₁S₁(l)

$S°(298.15 \text{ K}) = [82.811] \text{ J·K}^{-1}\text{·mol}^{-1}$ $\Delta_fH°(298.15 \text{ K}) = [-68.811] \text{ kJ·mol}^{-1}$

$T_{fus} = 1463 \pm 3 \text{ K}$ $\Delta_{fus}H° = 31.464 \pm 2.1 \text{ kJ·mol}^{-1}$

Enthalpy of Formation
$\Delta_fH°(\text{FeS, l, 298.15 K})$ is calculated from that of the crystal by adding the enthalpy of fusion, $\Delta_{fus}H°$, and the difference in enthalpy, $H°(1463 \text{ K})-H°(298.15 \text{ K})$, between the crystal and liquid.

Heat Capacity and Entropy
The heat capacity of liquid FeS above an assumed glass transition temperature of 1050 K is taken from Vaisburd and Zedina.[2] Their constant value of $C_p° = 14.95 \text{ cal·K}^{-1}\text{·mol}^{-1}$ is lower than $C_p° = 17.8 \text{ cal·K}^{-1}\text{·mol}^{-1}$ which we derive from the enthalpy data of Coughlin.[3] The latter value is based on two points separated by only 9 K while the results of Vaisburd and Zedina are quoted as covering the range from the mp to 1723 K. The heat capacity below the glass transition is that of the crystal.[1] $S°(\text{FeS, l, 298.15 K})$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data
The adopted melting point of 1463 ± 3 K is taken from the phase diagram of Hansen and Anderko.[4] The adopted enthalpy of fusion, $\Delta_{fus}H° = 7.52 \pm 0.5 \text{ kcal·mol}^{-1}$, is from our analysis of the high temperature enthalpy data of Coughlin.[3]

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_fH°$	$\Delta_fG°$	$\log K_f$
		J·K⁻¹·mol⁻¹			kJ·mol⁻¹		
0							
100							
200							
298.15	50.517	82.811	82.811	0.	-68.811	-75.798	13.280
300	50.671	83.124	82.812	0.094	-68.806	-75.842	13.205
400	89.203	101.550	85.057	6.597	-69.528	-78.222	10.215
411.000	95.051	104.049	85.532	7.610	ALPHA <--> BETA TRANSITION		
411.000	72.358	108.100	85.532	9.276	-67.190	-80.877	8.449
500	72.358	122.284	90.853	15.715	-66.248	-83.667	7.284
598.000	72.358	135.235	97.096	22.807	-66.837	-86.528	6.457
598.000	62.085	135.899	97.096	23.204	BETA <--> GAMMA TRANSITION		
600	62.030	136.106	97.226	23.328	-67.752	-89.283	5.830
700	59.808	145.489	103.472	29.412	-122.204	-90.818	5.271
800	58.560	153.383	109.230	35.332	-122.952	-87.300	4.560
900	58.286	160.255	114.526	41.156	-124.372	-83.648	3.972
1000	58.986	166.424	119.412	47.012	-125.094	-79.933	3.479
1050.000	59.702	169.318	121.720	49.978	-124.185	-76.207	3.062
1050.000	62.551	169.318	121.720	49.978	GLASS <--> LIQUID TRANSITION		
1100	62.551	172.228	123.950	53.106	-123.375	-72.548	2.707
1200	62.551	177.670	128.203	59.361			
1300	62.551	182.677	132.203	65.616			
1400	62.551	187.313	135.976	71.871			
1463.000	62.551	190.066	138.247	75.812			
1500	62.551	191.628	139.544	78.126	GAMMA <--> LIQUID TRANSITION		
1500	62.551	191.628	139.544	78.126	-122.664	-68.943	2.401
1600	62.551	195.665	142.927	84.381	-122.052	-65.382	2.134
1700	62.551	199.457	146.142	90.636	-122.487	-61.837	1.900
1800	62.551	203.033	149.204	96.891	-122.405	-58.273	1.691
1900	62.551	206.415	152.127	103.146	-136.518	-54.008	1.485
2000	62.551	209.623	154.922	109.401	-136.866	-49.656	1.297
2100	62.551	212.675	157.600	115.656	-137.226	-45.287	1.126
2200	62.551	215.585	160.170	121.911	-137.596	-40.900	0.971
2300	62.551	218.365	162.641	128.167	-137.975	-36.497	0.829
2400	62.551	221.027	165.018	134.422	-138.363	-32.076	0.698
2500	62.551	223.581	167.310	140.677	-138.759	-27.639	0.577
2600	62.551	226.034	169.522	146.932	-139.163	-23.187	0.466
2700	62.551	228.395	171.659	153.187	-139.572	-18.718	0.362
2800	62.551	230.670	173.726	159.442	-139.987	-14.235	0.266
2900	62.551	232.865	175.728	165.697	-140.408	-9.736	0.175
3000	62.551	234.985	177.668	171.952	-140.834	-5.223	0.091
3100	62.551	237.036	179.550	178.207	-141.265	-0.695	0.012
3200	62.551	239.022	181.378	184.462	-490.000	11.270	-0.184
3300	62.551	240.947	183.154	190.717	-488.538	26.912	-0.426
3400	62.551	242.814	184.881	196.972	-487.114	42.510	-0.653
3500	62.551	244.627	186.562	203.228	-485.727	58.067	-0.867
3600	62.551	246.389	188.200	209.483	-484.378	73.585	-1.068
3700	62.551	248.103	189.796	215.738	-483.069	89.066	-1.257
3800	62.551	249.771	191.352	221.993	-481.799	104.512	-1.437

Iron Sulfide, Troilite (FeS)

M_r = 87.907 Iron Sulfide, Troilite (FeS)

Fe₁S₁(cr,l)

CRYSTAL(α-β-γ)-LIQUID

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

T/K	C°_p	S°	-(G°-H°(T_r))/T	H°-H°(T_r)	Δ_f H°	Δ_f G°	log K_f
		J·K⁻¹·mol⁻¹			kJ·mol⁻¹		
0	0.	0.	INFINITE	-9.413	-102.166	-102.166	INFINITE
100	26.670	17.216	99.528	-8.231	-102.096	-101.959	53.258
200	43.052	41.665	64.714	-4.610	-101.886	-101.901	26.614
298.15	50.517	60.321	60.321	0.	-101.671	-101.953	17.862
300	50.671	60.634	60.322	0.094	-101.666	-101.954	17.752
400	89.203	79.060	62.567	6.597	-102.388	-102.086	13.331
411.000	95.051	81.559	63.042	7.610	ALPHA <--> BETA TRANSITION		
411.000	72.358	85.611	63.042	9.276			
500	72.358	99.794	68.363	15.715	-100.050	-102.492	10.707
598.000	72.358	112.745	74.607	22.807	BETA <--> GAMMA TRANSITION		
598.000	62.085	113.409	74.607	23.204			
600	62.030	113.617	74.736	23.328	-99.108	-103.033	8.970
700	59.808	122.999	80.982	29.412	-99.697	-103.645	7.734
800	58.560	130.893	86.740	35.322	-100.612	-104.151	6.800
900	58.286	137.765	92.036	41.156	-155.064	-103.437	6.003
1000	58.986	143.934	96.922	47.012	-155.812	-97.670	5.102
1100	60.662	149.627	101.457	52.986	-157.351	-91.766	4.358
1200	63.311	155.011	105.697	59.177	-158.138	-85.786	3.734
1300	66.935	160.216	109.692	65.681	-156.980	-79.802	3.206
1400	71.533	165.338	113.484	72.596	-155.509	-73.918	2.758
1463.000	74.930	168.560	115.786	77.208	GAMMA <--> LIQUID TRANSITION		
1463.000	62.551	190.066	115.786	108.671			
1500	62.551	191.628	117.638	110.986	-122.664	-68.943	2.401
1600	62.551	195.665	122.390	117.241	-122.052	-65.382	2.134
1700	62.551	199.457	126.813	123.496	-122.487	-61.837	1.900
1800	62.551	203.033	130.949	129.751	-122.405	-58.273	1.691
1900	62.551	206.415	134.832	136.006	-136.518	-54.008	1.485
2000	62.551	209.623	138.492	142.261	-136.866	-49.656	1.297
2100	62.551	212.675	141.953	148.516	-137.226	-45.287	1.126
2200	62.551	215.585	145.234	154.771	-137.596	-40.900	0.971
2300	62.551	218.365	148.354	161.026	-137.975	-36.496	0.829
2400	62.551	221.027	151.327	167.281	-138.363	-32.076	0.698
2500	62.551	223.581	154.166	173.537	-138.759	-27.639	0.577
2600	62.551	226.034	156.883	179.792	-139.163	-23.187	0.466
2700	62.551	228.395	159.489	186.047	-139.572	-18.718	0.362
2800	62.551	230.670	161.990	192.302	-139.987	-14.235	0.266
2900	62.551	232.865	164.397	198.557	-140.408	-9.736	0.175
3000	62.551	234.985	166.714	204.812	-140.834	-5.223	0.091
3100	62.551	237.036	168.950	211.067	-141.265	-0.695	0.012
3200	62.551	239.022	171.109	217.322	-490.000	11.270	-0.184
3300	62.551	240.947	173.196	223.577	-488.538	26.912	-0.426
3400	62.551	242.814	175.216	229.832	-487.114	42.510	-0.653
3500	62.551	244.627	177.174	236.087	-485.727	58.067	-0.867
3600	62.551	246.389	179.072	242.342	-484.378	73.585	-1.068
3700	62.551	248.103	180.915	248.597	-483.069	89.066	-1.257
3800	62.551	249.771	182.705	254.853	-481.799	104.512	-1.437

0   to   411   K   crystal, alpha
411 to   598   K   crystal, beta
598 to   1463 K   crystal, gamma
above   1463 K   liquid

Refer to the individual tables for details.

Iron Sulfide (FeS)   IDEAL GAS $M_r = 87.907$ Fe₁S₁(g)

$S°(298.15\ \text{K}) = 252.344 \pm 12.6\ \text{J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0\ \text{K}) = 370.49 \pm 16.3\ \text{kJ·mol}^{-1}$

$\Delta_f H°(298.15\ \text{K}) = 370.77 \pm 16.3\ \text{kJ·mol}^{-1}$

Electronic Levels and Quantum Weights

ϵ_i, cm⁻¹	g_i	ϵ_i, cm⁻¹	g_i	ϵ_i, cm⁻¹	g_i
[0]	[9]	[20481.9]	[9]	[30716.2]	[5]
[436.2]	[7]	[21462.2]	[9]	[30857.8]	[7]
[738.9]	[5]	[21699.9]	[7]	[30886.4]	[9]
[932.4]	[3]	[21857.2]	[5]	[34812.4]	[1]
[1027.3]	[1]	[24558.8]	[11]	[35803.7]	[5]
[19404.8]	[5]	[24940.9]	[9]	[40999.9]	[5]
[20688.4]	[3]	[25142.4]	[7]	[42896.9]	[7]
[21208.5]	[1]	[30088.8]	[7]	[49148.0]	[1]
[20051.1]	[13]	[30356.2]	[13]	[49576.9]	[3]
[20300.8]	[11]	[30725.8]	[3]	[50412.3]	[5]

$\omega_e = 550\ \text{cm}^{-1}$ $\omega_e x_e = [2.8]\ \text{cm}^{-1}$ $\sigma = 1$

$B_e = [0.198]\ \text{cm}^{-1}$ $\alpha_e = [0.0012]\ \text{cm}^{-1}$ $r_e = [2.05]\ \text{Å}$

Thermodynamic Table

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

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	J·K⁻¹·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	kJ·mol⁻¹	
0	0.	0.	INFINITE	-9.191	370.494	370.494	INFINITE
100	29.310	218.223	281.010	-6.279	372.294	352.331	-184.039
200	31.780	239.206	255.391	-3.237	371.925	332.401	-86.814
250	33.047	246.438	252.899	-1.615	371.390	322.579	-67.399
298.15	34.002	252.344	252.344	0.	370.767	313.234	-54.877
300	34.033	252.555	252.345	0.063	370.741	312.877	-54.477
350	34.775	257.860	252.762	1.784	370.010	303.289	-45.263
400	35.332	262.541	253.698	3.537	370.010	293.900	-38.379
450	35.756	266.728	254.917	5.315	366.991	284.847	-33.064
500	36.085	270.513	256.291	7.111	365.446	275.982	-28.832
600	36.554	277.137	259.229	10.745	363.784	258.710	-22.523
700	36.870	282.797	262.201	14.417	360.747	241.940	-18.054
800	37.095	287.736	265.091	18.116	357.746	225.607	-14.731
900	37.266	292.115	267.855	21.834	354.619	210.764	-12.232
1000	37.402	296.049	270.481	25.568	298.052	201.209	-10.510
1100	37.516	299.619	272.970	29.314	295.183	192.008	-9.118
1200	37.615	302.888	275.329	33.071	291.415	183.094	-7.970
1300	37.707	305.902	277.566	36.837	288.194	174.399	-7.007
1400	37.796	308.700	279.691	40.612	286.614	165.830	-6.187
1500	37.886	311.310	281.713	44.396	284.944	157.382	-5.481
1600	37.981	313.759	283.640	48.189	283.184	149.055	-4.866
1700	38.083	316.064	285.480	51.992	281.335	140.865	-4.328
1800	38.194	318.244	287.241	55.806	278.447	132.840	-3.855
1900	38.315	320.312	288.927	59.632	276.088	125.650	-3.454
2000	38.448	322.281	290.546	63.470	259.546	118.674	-3.099
2100	38.590	324.160	292.102	67.322	256.780	111.837	-2.782
2200	38.744	325.959	293.601	71.188	254.017	105.131	-2.496
2300	38.908	327.685	295.045	75.071	251.259	98.551	-2.238
2400	39.081	329.344	296.440	78.970	248.507	92.090	-2.004
2500	39.262	330.943	297.788	82.887	245.763	85.743	-1.791
2600	39.451	332.487	299.093	86.823	243.029	79.505	-1.597
2700	39.645	333.979	300.358	90.778	240.307	73.372	-1.449
2800	39.844	335.425	301.585	94.752	237.597	67.339	-1.256
2900	40.046	336.826	302.776	98.746	234.901	61.402	-1.106
3000	40.251	338.188	303.934	102.761	232.220	55.557	-0.967
3100	40.456	339.511	305.060	106.797	229.553	49.801	-0.839
3200	40.662	340.798	306.157	110.852	226.903	51.554	-0.842
3300	40.866	342.053	307.226	114.929	-124.031	57.052	-0.903
3400	41.069	343.276	308.268	119.026	-124.748	62.572	-0.961
3500	41.270	344.469	309.286	123.143	-125.482	68.114	-1.017
3600	41.467	345.634	310.279	127.279	-126.234	73.678	-1.069
3700	41.659	346.773	311.250	131.436	-127.003	79.263	-1.119
3800	41.848	347.887	312.200	135.611	-127.792	84.870	-1.167
3900	42.031	348.976	313.129	139.805	-128.602	90.499	-1.212
4000	42.209	350.043	314.038	144.017	-129.434	96.149	-1.256
4100	42.382	351.087	314.929	148.247	-130.290	101.820	-1.297
4200	42.548	352.110	315.802	152.494	-131.171	107.514	-1.337
4300	42.709	353.113	316.658	156.756	-132.080	113.230	-1.375
4400	42.863	354.097	317.498	161.035	-133.018	118.968	-1.412
4500	43.011	355.062	318.322	165.329	-133.987	124.728	-1.448
4600	43.153	356.009	319.131	169.637	-134.989	130.511	-1.482
4700	43.288	356.938	319.926	173.959	-136.025	136.316	-1.515
4800	43.417	357.851	320.706	178.294	-137.099	142.145	-1.547
4900	43.540	358.748	321.474	182.642	-138.211	147.998	-1.578
5000	43.656	359.628	322.228	187.002	-139.363	153.875	-1.608
5100	43.767	360.494	322.970	191.373	-140.559	159.776	-1.636
5200	43.872	361.345	323.700	195.755	-141.799	165.701	-1.664
5300	43.971	362.182	324.418	200.148	-143.087	171.652	-1.692
5400	44.065	363.004	325.125	204.549	-144.423	177.629	-1.718
5500	44.153	363.814	325.821	208.960	-145.811	183.631	-1.744
5600	44.236	364.610	326.506	213.380	-147.253	189.661	-1.769
5700	44.314	365.394	327.182	217.807	-148.751	195.718	-1.794
5800	44.387	366.165	327.847	222.243	-150.309	201.803	-1.817
5900	44.456	366.924	328.503	226.685	-151.928	207.916	-1.841
6000	44.521	367.672	329.150	231.134	-153.612	214.058	-1.864

PREVIOUS September 1977 (1 atm)   CURRENT: September 1977 (1 bar)

Enthalpy of Formation

Drowart et al.[1] used a modified Knudsen cell and a mass spectrometric technique to study the equilibrium FeS(g) + Mn(g) = MnS(g) + Fe(g). We adopt a value of $D_0°$ = 76.3 ± 3.5 kcal·mol⁻¹ based on their 3rd law analysis of this equilibrium. With auxiliary JANAF data[2] this yields $\Delta_f H°$(298.15 K) = 88.6 ± 3.9 kcal·mol⁻¹. Trevedi[3] studied the absorption spectrum of FeS and determined $D_0°$ = 93 kcal·mol⁻¹ from the onset of continuous absorption due to photodissociation. This value is likely to be too high in view of the experimental difficulties in determining the exact position of the onset of continuous absorption. Complications arise because of background emission from the furnace. Marquardt and Berkowitz[4] determined an upper limit $D_0°$ < 77 kcal·mol⁻¹ by mass-spectrometric measurements. These results may be biased since they used ν = 412 cm⁻¹ for the vibrational frequency of FeS in determining their Gibbs energy functions. A Birge–Sponer extrapolation of the vibrational data to determine $D_0°$ is not meaningful since DeVore and Franzen[5] used the reverse procedure to arrive at the reported value of $\omega_e x_e$.

Heat Capacity and Entropy

With the exception of the observance of one excited state at 17992 cm⁻¹ with a vibrational spacing of ~497 cm⁻¹ by DeVore and Franzen,[5] there is no information on the electronic spectrum of FeS(g). The identity and quantum weight of this state, as well as the ground state, are unknown. As a result, the electronic states are estimated to be identical to those of the Fe²⁺ ion[6] following the procedure of Brewer and Rosenblatt[7] for the transition metal oxides. As stated by Brewer and Rosenblatt,[7] this procedure usually overestimates the contribution of electronic states. Nevertheless; it appears to be the best method available. The uncertainty assigned to S°(298.15 K) is based mainly on the uncertainties in this approximation since the presence of the sulfide ion will undoubtedly alter the electronic structure of the iron ion. Levels above 50,000 cm⁻¹ are not included since they have a negligible effect on the thermodynamic properties. The vibrational constants are taken from a study of the matrix isolation spectrum by DeVore and Franzen.[5] The rotational constants are estimated based on an oxide–sulfide correlation due to Barrow and Cousins,[8] r(FeS) = 0.237 ± 1.116 r(FeO). The value r(FeO) = 1.626 Å is taken from Suchard.[9] The value of α_e is estimated assuming a Morse potential function using the expression given by Herzberg.[10]

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Iron Sulfide (FeS)   Fe₁S₁(g)

Iron Sulfide, Marcasite (FeS₂)   CRYSTAL M_r = 119.967   Iron Sulfide, Marcasite (FeS₂)   Fe₁S₂(cr)

$S°(298.15 \text{ K}) = 53.865 \pm 0.13 \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = -163.78 \pm 2.1 \text{ kJ·mol}^{-1}$

$\Delta_f H°(298.15 \text{ K}) = -167.36 \pm 2.1 \text{ kJ·mol}^{-1}$

| | Enthalpy Reference Temperature = T_r = 298.15 K | | | | Standard State Pressure = $p°$ = 0.1 MPa | | |
| | J·K⁻¹·mol⁻¹ | | | | kJ·mol⁻¹ | | |
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	-9.753	-163.782	-163.782	INFINITE
100	19.269	7.576	99.375	-9.180	-163.012	-162.658	84.964
200	49.399	31.380	59.227	-5.569	-166.454	-159.685	41.705
298.15	62.390	53.865	53.865	0.	-167.360	-156.159	27.358
300	62.554	54.251	53.866	0.116	-167.375	-156.090	27.178
400	69.169	73.244	56.411	6.733	-172.579	-152.034	19.854
500	72.447	89.075	61.407	13.834	-176.187	-145.504	15.305
600	74.568	102.472	67.163	21.185	-179.092	-140.283	12.213
700	76.959	114.139	73.058	28.757	-181.539	-133.617	9.971
800	78.668	124.569	78.857	36.569	-183.764	-126.619	8.267
900	80.718	133.953	84.466	44.538	-292.337	-117.177	6.801
1000	82.764	142.563	89.851	52.712	-292.623	-97.707	5.104
1100	84.810	150.547	95.010	61.091	-293.630	-78.151	3.711
1200	86.860	158.014	99.952	69.674	-293.910	-58.568	2.549
1300	88.910	165.048	104.692	78.463	-292.370	-39.018	1.568
1400	90.960	171.712	109.243	87.456	-290.740	-19.589	0.731

Enthalpy of Formation

Based on highly accurate adiabatic-shield calorimetry measurements, Gronvold and Westrum[1] reported that the enthalpy of transformation of marcasite to pyrite is -1.05 ± 0.05 kcal·mol⁻¹ at 700 K. The adopted value of $\Delta_f H°$(298.15 K) is selected to reproduce this enthalpy of reaction within the reported uncertainty. Lipin et al.[2] based on combustion calorimetry, reported a value of -5.6 kcal·mol⁻¹ for the marcasite pyrite transformation at 298.15 K. Due to the state of the art in combustion calorimetry at the time of this measurement and uncertainty in the products (oxides of sulfur), this value must have a high uncertainty and is given no weight in our selection process.

Heat Capacity and Entropy

The adopted heat capacities of marcasite are based on our analysis of the $C_p°$ measurements (6–700 K) of Gronvold and Westrum.[1] Values above 700 K are extrapolated assuming $C_p°$(marcasite) + 0.075 cal·K⁻¹·mol⁻¹.

The adopted value of $S°$(298.15 K) is obtained from the appropriate integration of the adopted $C_p°$ data assuming $S°$(6.06 K) = 0.0008 cal·K⁻¹·mol⁻¹.

Phase Data

Marcasite has an orthorhombic structure, V_h^{12} = Pnnm, and exists as stoichiometric FeS₂ within the limits of experimental error.[3] Marcasite is known to be metastable with respect to the other known FeS₂ polymorph, cubic pyrite, above 673 K[3] the JANAF Thermochemical Tables[4] indicate it will also be metastable below 673 K. The marcasite to pyrite transformation is kinetically slow at low temperatures and this accounts for the persistence of marcasite in nature. Kjekshus and Rakke[5] found no conversion to pyrite using heat treatments at 573 K for periods up to 14 months. At 673 K the conversion to pyrite is complete in 4 months and is even more rapid (< 1 hour) at 973 K[5]. Indications are that the conversion to pyrite will be complete before the pyrite decomposition temperature of 1016 K is reached.[3]

References

[1] F. Gronvold and E. F. Westrum, J. Chem. Thermodyn. 8, 1039 (1976).
[2] S. V. Lipin, V. S. Uskov and V. R. Klokman, Zhur. Prikl. Khim. 15, 411 (1942).
[3] G. Kullerud and H. S. Yoder, Econ. Geol. 54, 533 (1959).
[4] JANAF Thermochemical Tables: FeS₂(cr, pyrite) 9-30-77.
[5] A. Kjekshus and T. Rakke, Acta Chem. Scand. Ser. A A29, 443 (1975).

Iron Sulfide, Pyrite (FeS₂)   CRYSTAL M_r = 119.967

$$S°(298.15 \text{ K}) = 52.916 \pm 0.13 \text{ J·K}^{-1}\text{·mol}^{-1}$$

$$\Delta_f H°(0 \text{ K}) = -167.86 \pm 2.1 \text{ kJ·mol}^{-1}$$
$$\Delta_f H°(298.15 \text{ K}) = -171.54 \pm 2.1 \text{ kJ·mol}^{-1}$$

Enthalpy of Formation

The adopted value of $\Delta_f H°(298\ 15 \text{ K}) = -41.0 \pm 0.5$ kcal mol⁻¹ is based on our 3rd law analysis of the equilibrium data of Toulmin and Barton.[1] These authors made corrections for the changing stoichiometry of pyrrhotite as a function of temperature in the pyrrhotite–pyrite equilibrium, and also accounted for the changing activity of pyrite as a function of temperature and stoichiometry These corrections have not been applied to our analysis of the rest of the equilibrium data shown below

Source	Method	Reaction*	T/K	Data Points	$\Delta_f H°$(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
Toulmin[1]	Electrum–tarnish	A	598–1016	17**	-71.77 ± 0.12	71.89 ± 0.16	-0.15 ± 0.15	41.0 ± 0.5
DeRudder[2]	Manometric	B	873–962	7	-32.47 ± 1.27	-27.74 ± 0.43	5.17 ± 1.38	43.2 ± 0.6
Ugai[3]	Gravimetric	B	923–1016	equation	-16.70	-26.81 ± 0.93	-10.28	36.0
DeRanter[4]	emf	C	298.15	1		-36.00		42.3 ± 1.0
Schneeberg[5]	emf	B	597–711	4	-28.98 ± 1.10	28 16 ± 0.26	1.26 ± 1.68	43.6 ± 0.5
Rosenqvist[6]	Dew point	B	869–1030	22	-34.03 ± 1.22	-28.04 ± 0.63	6.35 ± 1.29	43.5 ± 0.7

**Point at 1009 K rejected by statistical test.

*Reaction: (A) $Fe(cr) + S_2(g) \rightarrow FeS_2(cr, pyrite)$
(B) $1.14\ Fe_{0.877}S(cr) + 0\ 43\ S_2(g) \rightarrow FeS_2(cr, pyrite)$
(C) $Fe(cr) + 2\ S(cr) \rightarrow FeS_2(cr, pyrite)$.

The value reported by DeRanter[4] is biased since FeS₂ is a semiconductor and DeRanter acknowledged that semiconductors lead to incorrect results in his emf technique. The other values are believed to be biased because the equilibrium is treated as if the composition ($Fe_{0.877}S$) and activity (a=1) of pyrrhotite remain unchanged.

Heat Capacity and Entropy

The adopted values of $C_p°$ are based on our analysis of the calorimetrically measured values of Gronvold and Westrum, 4–346 K[7] and 314–688 K.[8] At higher temperatures the $C_p°$ values are based on our analysis of the enthalpy data of Coughlin,[9] 405–980 K, which merges smoothly with the $C_p°$ data of Gronvold and Westrum. Values above 980 K are extrapolated.

The adopted value of $S°(298.15 \text{ K})$ is obtained from the appropriate integration of the adopted $C_p°$ data assuming $S°(4.6 \text{ K}) = 0.0007$ cal·K⁻¹·mol⁻¹.

Phase Data

Pyrite has a cubic structure, T_h^6 - Pa3, and exits as stoichiometric FeS₂ within the limits of experimental error.[10] The other known FeS₂ polymorph is orthorhombic marcasite which is known to be metastable with respect to pyrite above 673 K[10] the JANAF Thermochemical Tables[11] indicate that pyrite will also be the stable form below 673 K.

Decomposition Data

Pyrite melts incongruently to pyrrhotite, a liquid whose composition is ~FeS₄[3] and vapor at 1016 ± 2 K at the vapor pressure of the system, 10 atm.[3][10] Assuming the vapor to be composed only of S₂(g), we calculate[11] a decomposition temperature of 906 K at 1 atm for the process

$$2.3263\ FeS_2(pyrite) \rightarrow S_2(g) + 2.6525\ Fe_{0.877}S(cr).$$

References

[1] P. Toulmin and P. B. Barton, Geochim. Cosmochim. Acta 28, 641 (1964).
[2] F. DeRudder, Bull. Soc. Chim. Fr. 47, 1225 (1930).
[3] Y. A. Ugai, V. Z. Anokhin, A. N. Prokin and V. R. Pshestanchik, Irv. Akad. Nauk SSSR, Neorg. Mater. 10, 250 (1974).
[4] C. DeRanter and R. Breckpot, Bull. Soc Chim. Belg 78, 503 (1969).
[5] E. P. Schneeberg, Econ. Geol. 68. 507 (1973).
[6] T. Rosenqvist, J. Iron Steel Inst. (London) 176, 37 (1957).
[7] F. Gronvold and E. F. Westrum, Inorg. Chem. 1, 36 (1962).
[8] F. Gronvold and E. F. Westrum, J. Chem. Thermodyn. 8, 1039 (1976).
[9] J. P. Coughlin, J. Amer. Chem. Soc. 72, 5445 (1950).
[10] G. Kullend and H. S. Yoder, Econ. Geol. S4, 533 (1959).
[11] JANAF Thermochemical Tables: FeS₂(cr, marcasite), 9-30-77; Fe₀.₈₇₇S(cr), 9-30-77.

Iron Sulfide, Pyrite (FeS₂)   Fe₁S₂(cr)

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	-9.641	-167.855	-167.855	INFINITE
100	18.712	7.091	98.120	-9.103	-169.119	-166.717	87.084
200	49.056	30.556	58.251	-5.539	-170.607	-163.674	42.747
298.15	62.124	52.916	52.916	0.	-171.544	-160.060	28.042
300	62.289	53.301	52.918	0.115	-171.559	-159.989	27.857
400	68.848	72.213	55.451	6.705	-176.792	-155.835	20.350
500	72.040	87.953	60.425	13.764	-180.441	-150.197	15.691
600	74.307	101.295	66.152	21.086	-183.375	-143.860	12.524
700	76.308	112.899	72.019	28.616	-185.865	-137.074	10.229
800	78.354	123.222	77.786	36.349	-188.169	-129.946	8.485
900	80.404	132.569	83.362	44.287	-296.773	-120.367	6.986
1000	82.450	141.146	88.717	52.429	-297.090	-100.757	5.263
1100	84.496	149.101	93.849	60.777	-298.128	-81.058	3.849
1200	86.546	156.541	98.767	69.329	-298.440	-61.329	2.670
1300	88.592	163.549	103.483	78.086	-296.931	-41.630	1.673
1400	90.642	170.189	108.012	87.047	-295.333	-22.051	0.823

CURRENT: September 1977

Iron Iodine ((FeI₂)₂)　　　　　　**IDEAL GAS**　　　　$M_r = 619.3120$ Iron Iodide ((FeI₂)₂)　　　　　　Fe₂I₄(g)

$S°(298.15 \text{ K}) = [543.471] \text{ J·K}^{-1}\text{·mol}^{-1}$

$\Delta_f H°(0 \text{ K}) = 9.75 \pm 20.9 \text{ kJ·mol}^{-1}$
$\Delta_f H°(298.15 \text{ K}) = 8.37 \pm 20.9 \text{ kJ·mol}^{-1}$

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	-34.030	9.747	9.747	INFINITE
100	119.470	404.580	658.433	-25.385	11.447	-15.500	8.149
200	129.233	491.411	555.431	-12.804	10.625	-42.494	11.098
250	130.564	520.408	545.629	-6.305	9.593	-55.661	11.630
298.15	131.283	543.471	543.471	0.	8.368	-68.121	11.935
300	131.304	544.284	543.474	0.243	8.316	-68.596	11.944
350	131.756	564.561	545.074	6.820	6.698	-81.293	12.132
400	132.052	582.175	548.635	13.416	-27.043	-92.647	12.098
450	132.258	597.741	553.243	20.024	-31.296	-100.593	11.676
500	132.409	611.684	558.402	26.641	-115.916	-100.461	10.495
600	132.629	635.845	569.357	39.893	-116.344	-97.338	8.474
700	132.820	656.305	580.354	53.166	-117.258	-94.105	7.022
800	133.038	674.054	590.981	66.458	-118.753	-90.704	5.922
900	133.308	689.739	601.100	79.775	-121.074	-87.069	5.053
1000	133.635	703.800	610.679	93.122	-124.826	-83.108	4.341
1100	134.013	716.555	619.733	106.504	-130.359	-78.640	3.734
1200	134.430	728.233	628.295	119.926	-134.783	-73.781	3.212
1300	134.872	739.010	636.402	133.391	-135.917	-68.653	2.759
1400	135.325	749.022	644.093	146.900	-137.235	-63.431	2.367
1500	135.774	758.374	651.404	160.455	-138.756	-58.107	2.023
1600	136.209	767.150	658.366	174.055	-140.500	-52.675	1.720
1700	136.620	775.421	665.011	187.696	-144.386	-47.089	1.447
1800	137.001	783.240	671.364	201.378	-147.300	-41.283	1.198
1900	137.347	790.657	677.449	215.095	-178.679	-33.904	0.932
2000	137.655	797.710	683.287	228.846	-182.614	-26.182	0.684
2100	137.924	804.433	688.897	242.625	-186.656	-18.262	0.454
2200	138.153	810.855	694.296	256.429	-190.797	-10.147	0.241
2300	138.345	817.000	699.498	270.254	-195.027	-1.841	0.042
2400	138.500	822.891	704.518	284.097	-199.330	6.651	-0.145
2500	138.621	828.548	709.367	297.953	-203.686	15.322	-0.320
2600	138.710	833.987	714.056	311.820	-208.077	24.170	-0.486
2700	138.771	839.223	718.595	325.694	-212.481	33.186	-0.642
2800	138.806	844.270	722.994	339.573	-216.879	42.365	-0.790
2900	138.817	849.141	727.260	353.455	-221.251	51.701	-0.931
3000	138.808	853.847	731.402	367.334	-225.581	61.187	-1.065
3100	138.782	858.398	735.426	381.216	-229.853	70.817	-1.193
3200	138.740	862.804	739.338	395.092	-930.654	95.431	-1.558
3300	138.685	867.072	743.144	408.963	-930.973	127.501	-2.018
3400	138.618	871.212	746.850	422.829	-931.267	159.580	-2.452
3500	138.543	875.229	750.461	436.687	-931.529	191.668	-2.860
3600	138.459	879.130	753.981	450.537	-931.758	223.762	-3.247
3700	138.369	882.923	757.415	464.378	-931.950	255.863	-3.612
3800	138.275	886.612	760.767	478.211	-932.106	287.969	-3.958
3900	138.176	890.202	764.040	492.033	-932.225	320.078	-4.287
4000	138.074	893.699	767.238	505.846	-932.311	352.189	-4.599
4100	137.970	897.107	770.364	519.648	-932.365	384.302	-4.896
4200	137.865	900.431	773.421	533.440	-932.392	416.416	-5.179
4300	137.760	903.674	776.413	547.221	-932.396	448.531	-5.449
4400	137.654	906.839	779.341	560.992	-932.380	480.645	-5.706
4500	137.549	909.932	782.209	574.752	-932.351	512.759	-5.952
4600	137.444	912.954	785.019	588.501	-932.312	544.872	-6.187
4700	137.340	915.909	787.772	602.241	-932.270	576.984	-6.412
4800	137.238	918.799	790.472	615.969	-932.197	609.096	-6.628
4900	137.137	921.628	793.120	629.688	-932.197	641.207	-6.835
5000	137.038	924.397	795.718	643.397	-932.178	673.316	-7.034
5100	136.941	927.110	798.268	657.096	-932.178	705.427	-7.225
5200	136.845	929.768	800.771	670.785	-932.204	737.537	-7.409
5300	136.752	932.374	803.230	684.465	-932.250	769.647	-7.585
5400	136.661	934.929	805.645	698.136	-932.354	801.760	-7.755
5500	136.572	937.436	808.018	711.797	-932.492	833.874	-7.919
5600	136.486	939.896	810.351	725.450	-932.681	865.992	-8.078
5700	136.401	942.311	812.645	739.094	-932.927	898.113	-8.230
5800	136.319	944.683	814.902	752.730	-933.238	930.239	-8.378
5900	136.239	947.012	817.121	766.358	-933.621	962.371	-8.520
6000	136.161	949.301	819.305	779.978	-934.083	994.510	-8.658

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

Iron Iodide ((FeI₂)₂)　　　　　Fe₂I₄(g)

Electronic Levels and Quantum Weights

ϵ, cm⁻¹	g_i
0	[5]
[4200]	[5]
[6800]	[5]

Vibrational Frequencies and Degeneracies

ν, cm⁻¹	ν, cm⁻¹	ν, cm⁻¹
[100](1)	[70](1)	[80](2)
[50](1)	[90](1)	[20](2)
[95](1)	[105](1)	[160](2)

Point Group: [D₂ₕ]　　　　$\sigma = 4$
Bond Distance: Fe–I = [2.43] Å
Bond Angles: I–Fe–I_bridge = [135]°　Fe–I_bridge–Fe = [90]°　I_bridge–Fe–I_bridge = [90]°
Product of the Moments of Inertia: $I_A I_B I_C = [8.778988 \times 10^{-110}] \text{ g}^3\text{·cm}^6$

Enthalpy of Formation

The chemical equilibrium of the interaction of Fe(cr) and I(g) has been studied by a transpiration method by Zaugg and Gregory.[1] Using the reported equilibrium constants in the temperature range from 591 to 751 K, the enthalpy change $\Delta_f H°(298.15 \text{ K})$ of the reaction 2Fe(cr) + 4I(g) = Fe₂I₄(g) was evaluated by both the 2nd and 3rd law method to be -85.3 and -103.75 kcal·mol⁻¹, respectively. The corresponding values of the enthalpy of formation, $\Delta_f H°$(Fe₂I₄, g, 298.15 K), are calculated as +16.9 and -1.6 kcal·mol⁻¹. Mass spectrometric and Knudsen effusion techniques have been used to study the vaporization of FeI₂(cr) by Schoonmaker et al.[2] Using the reported vapor pressure, $p = 1.21 \times 10^{-6}$ atm at 714 K for Fe₂I₄(g), the enthalpy change $\Delta_f H°(298.15 \text{ K})$ for the reaction 2FeI₂(cr) = Fe₂I₄(g) was evaluated by the 3rd law method as 52.8 kcal·mol⁻¹, yielding $\Delta_f H°(298.15 \text{ K})$ = 2.8 kcal·mol⁻¹ for Fe₂I₄(g).
The adopted value of $\Delta_f H°(298.15 \text{ K})$ for Fe₂I₄(g) is 2.0 ± 5 kcal·mol⁻¹ (8.368 ± 20.9 kJ·mol⁻¹).

Heat Capacity and Entropy

The molecular structure was assumed to be the same as that for Fe₂Br₄(g). The Fe–I bond distance was estimated from that in FeI₂(g). The four vibrational frequencies (ν_i), i.e. i = 2, 4, 5 and 6, were estimated by comparison with those for K₂I₂(g), calculated by Berkowitz.[3] The other frequency values were estimated from those for FeI₂(g). The electronic levels and quantum weights were estimated from those for FeI₂(g). The principal moments of inertia are: $I_A = 124.4358 \times 10^{-39}$, $I_B = 780.0258 \times 10^{-39}$, and $I_C = 904.4616 \times 10^{-39}$ g·cm².

References

[1] W. E. Zaugg and N. W. Gregory, J. Phys. Chem. 70, 490 (1966).
[2] R. C. Schoonmaker, A. H. Friedman and R. F. Porter, J. Chem. Phys. 31, 1585 (1959).
[3] J. Berkowitz, J. Chem. Phys. 32, 1519 (1960).

Iron Oxide, Hematite (Fe₂O₃)   **CRYSTAL** $M_r = 159.6922$ Iron Oxide, Hematite (Fe₂O₃)   Fe₂O₃(cr)

$S°(298.15\ K) = 87.400\ J\cdot K^{-1}\cdot mol^{-1}$

$\Delta_f H°(0\ K) = -819.03 \pm 1.3\ kJ\cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -825.50 \pm 1.3\ kJ\cdot mol^{-1}$

		Enthalpy Reference Temperature = T_r = 298.15 K			Standard State Pressure = $p°$ = 0.1 MPa		
		J·K⁻¹·mol⁻¹			kJ·mol⁻¹		
T/K	$C°_p$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	-15.560	-819.025	-819.025	INFINITE
100	31.497	14.611	159.795	-14.518	-823.186	-797.438	416.539
200	76.567	51.279	96.132	-8.970	-825.542	-770.573	201.253
298.15	103.763	87.400	87.400	0.	-825.503	-743.523	130.262
300	104.182	88.043	87.402	0.192	-825.485	-743.014	129.370
400	120.123	120.299	91.691	11.443	-823.947	-715.727	93.464
500	131.796	148.400	100.284	24.058	-821.626	-688.929	71.972
600	141.168	173.270	110.415	37.713	-818.882	-662.642	57.688
700	149.729	195.675	121.020	52.259	-815.870	-636.837	47.521
800	158.218	216.225	131.653	67.658	-812.705	-611.477	39.925
900	166.490	235.340	142.124	83.894	-809.634	-585.510	34.040
950.000	170.570	244.451	147.271	92.321		I <--> II TRANSITION	
950.000	150.624	245.156	147.271	92.990			
1000	150.624	252.882	152.360	100.522	-807.695	-561.866	29.349
1050.000	150.624	260.231	157.323	108.053		II <--> III TRANSITION	
1050.000	140.407	260.231	157.323	108.053			
1100	140.775	266.771	162.150	115.083	-809.682	-537.171	25.508
1200	141.511	279.052	171.388	129.197	-811.071	-512.374	22.303
1300	142.248	290.408	180.112	143.385	-809.145	-487.562	19.590
1400	142.984	300.976	188.372	157.647	-807.358	-462.893	17.271
1500	143.720	310.866	196.212	171.982	-805.706	-438.347	15.265
1600	144.566	320.170	203.671	186.397	-804.180	-413.906	13.513
1700	145.266	328.956	210.785	200.890	-804.681	-389.520	11.968
1800	145.780	337.275	217.583	215.445	-804.094	-365.117	10.595
1900	146.231	345.169	224.092	230.045	-831.859	-339.338	9.329
2000	146.789	352.684	230.335	244.696	-832.056	-313.410	8.185
2100	147.277	359.858	236.334	259.400	-832.235	-287.474	7.151
2200	147.695	366.719	242.105	274.149	-832.403	-261.528	6.209
2300	148.044	373.292	247.667	288.937	-832.566	-235.576	5.350
2400	148.323	379.599	253.034	303.756	-832.731	-209.617	4.562
2500	148.532	385.658	258.219	318.599	-832.905	-183.650	3.837

PREVIOUS: CURRENT: June 1965

Enthalpy of Formation

The chemical equilibria for the reaction 4 Fe₃O₄(cr) + O₂(g) = 6 Fe₂O₃(cr) have been studied by several investigators. From the reported data the corresponding values of $\Delta_r H°$(298.15 K) and $\Delta_f H°$(Fe₂O₃, cr, 298.15 K) were evaluated. The results obtained are given as follows:

Source	T/K	$\Delta_r H°$(298.15 K), kcal·mol⁻¹ 2nd law	3rd law	$\Delta_f H°$(298.15 K) kcal·mol⁻¹
Tretyakov and Khomyakov[1]	1373–1728	-106.32 ± 0.19	-111.05	-197.11
Schmahl[2]	1583–1683	-123.95 ± 1.37	-112.94	-197.42
Smiltens[3]	1373–1673	-117.88 ± 0.38	-114.25	-197.64
Darken and Gurry[4]	1723		-110.29	196.98

The value of $\Delta_f H°$(298.15 K) adopted for Fe₂O₃(cr) is the weighted average of the $\Delta_f H°$(298.15 K) values listed in the above table.

Heat Capacity and Entropy

The low temperature (5.58-345.42 K) heat capacities were determined by Gronvold and Westrum.[5] The high temperature (298-1750 K) $C°_p$ values were obtained from Coughlin et al.[6] The two sets of data were plotted and joined smoothly at 298 K. The $C°_p$ values above 1750 K were obtained by graphical extrapolation. The heat capacities of Fe₂O₃(cr) have also been reported by Brown and Furnas (0-650 °C),[7] and Parks and Kelley (88 289 K).[8] $S°$(298.15 K) for Fe₂O₃(cr) was derived from the smoothed $C°_p$ data, based on $S°$(5 K) = 0.0003 cal·K⁻¹·mol⁻¹. Coughlin et al.[6] measured the enthalpy for hematite and found two anomalies, presumably of magnetic nature, at about 950 and 1050 K, respectively. Both appear to involve maxima in the heat capacity curves rather than isothermal heats of transformation. The complex magnetic properties at low temperatures were discussed by Gronvold and Westrum.[5] No heat capacity anomaly was observed at the magnetic transition about 250 K. The Curie points of the antiferromagnetic α-Fe₂O₃ were reported by Aharoni et al.[9] and Lielmezs and Chaklader.[10]

Decomposition Data

T_{dcm} = 1735 K is the temperature at which the pressure is 1 atm for the reaction 6 Fe₂O₃(cr) = 4 Fe₃O₄(cr) + O₂(g). In other words, Fe₂O₃(cr) decomposes into Fe₃O₄(cr) and O₂(g) at 1735 K.

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Iron Sulfate (Fe2(SO4)3)   CRYSTAL $M_r = 399.8668$ Fe2O12S3(cr)

$S°(298.15 \text{ K}) = [307.524 \pm 8.4] \text{ J·K}^{-1}\text{·mol}^{-1}$

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

$\Delta_f H°(298.15 \text{ K}) = -2582.99 \pm 1.67 \text{ kJ·mol}^{-1}$

Enthalpy of Formation

The enthalpy change, $\Delta_f H°(298.15 \text{ K})$, for the chemical reaction $Fe_2O_3(cr) + 3(H_2SO_4\cdot14.855\ H_2O)(sol.) = Fe_2(SO_4)_3(cr) + 47.565\ H_2O(l)$ was measured to be 8.54 + 0.18 kcal·mol⁻¹ by solution calorimetry by Barany and Adami.[1] Using $\Delta_f H°(298.15 \text{ K})$ for $H_2SO_4\cdot14.855\ H_2O$(sol.) and -68.315 kcal·mol⁻¹ for H_2O(l), obtained from and -197.3 kcal·mol⁻¹ for Fe_2O_3(cr), the enthalpy of formation, $\Delta_f H°(298.15 \text{ K})$, for $Fe_2(SO_4)_3$(cr) was evaluated as -617.35 ± 0.40 kcal·mol⁻¹ which was adopted here.

The equilibrium pressures for the decomposition of $Fe_2(SO_4)_3$(cr) have been determined by several investigators at different temperatures. The chemical reactions are: (1) $Fe_2(SO_4)_3$(cr) $= Fe_2O_3$(cr) $+ 3\ SO_3$(g) and (2) SO_3(g) $= SO_2$(g) $+ 0.5\ O_2$(g). However, the measured pressure of the chemical equilibrium is the total pressure of three partial pressures, namely, P(SO₃), P(SO₂), and P(O₂). In order to calculate the enthalpy change of Reaction (1), the partial pressures of SO₃(g) were evaluated from the total vapor pressure data at each temperature. Based on the derived values for P(SO₃), the $\Delta_f H°(298.15 \text{ K})$ value for Reaction (1) was calculated by both the 2nd and 3rd law methods. The results obtained are presented in the following table. The $\Delta_f H°(Fe_2(SO_4)_3$, cr, 298.15 K) values were derived, using the 3rd law and 2nd law $\Delta_f H°(298.15 \text{ K})$. These determinations were not given any weight.

Source	T/K	$\Delta_f H°$(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
Keppeler and D'Ans[3]	753.15–1013.15	136.8 ± 0.5	139.9 ± 0.5	3.4 ± 0.6	-621.0
Wohler, et al.[4]	826.15– 980.15	114.2 ± 6.2	133.1 ± 2.3	19.2 ± 6.9	-614.2
Bodenstein and Suzuki[5]	903.65– 997.15	140.7 ± 6.6	139.1 ± 1.3	-1.2 ± 7.1	-620.2
Wohler and Grunzweig[6]	909.15– 994.15	155.1 ± 1.3	135.5 ± 1.3	-20.4 ± 1.4	-616.6
Neumann and Heintke[7]	793 15– 973.15	136.4 ± 2.3	136.2 ± 1.2	-1.2 ± 2.6	-617.3
Warner and Ingraham[8]	903.15– 997.15	133.9 ± 2.6	135.4 ± 0.5	1.7 ± 2.7	-616.5

The decomposition pressures of $Fe_2(SO_4)_3$(cr) have also been investigated by: Grunzweig (793–994 K),[9] Blanks (845–976 K),[10] and Ingraham (856–995 K).[11] These data together with some of the data mentioned previously were critically reviewed by Kellogg.[12]

Heat Capacity and Entropy

The heat capacities were estimated by comparison with those for FeSO₄(cr), assuming their average specific heats, cal·K⁻¹·g⁻¹, to be the same. The value of $S°(298.15 \text{ K})$ was estimated so that the 2nd and 3rd law $\Delta_f H°(298.15 \text{ K})$ values, derived from decomposition pressure data, are in reasonable agreement.

Decomposition Data

T_{dcm} is the temperature (1451 K) at which the total pressure of the gaseous products equals one atmosphere, which was obtained by graphical extrapolation of the decomposition pressure data measured by Warner and Ingraham.[8]

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Iron Sulfate (Fe2(SO4)3)

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

T/K	$C_p°$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹·mol⁻¹				kJ·mol⁻¹		
0							
100							
200							
298.15	264.722	307.524	307.524	0.	-2582.992	-2262.729	396.421
300	265.851	309.165	307.529	0.491	-2583.047	-2260.742	393.630
400	307.022	391.497	318.475	29.209	-2591.203	-2152.742	281.119
500	339.281	463.626	340.441	61.593	-2594.662	-2042.719	213.401
600	363.297	527.707	366.413	96.776	-2595.362	-1932.225	168.215
700	380.702	585.079	393.626	134.017	-2594.341	-1821.767	135.942
800	393.254	636.776	420.843	172.746	-2592.496	-1711.521	111.751
900	402.041	683.617	447.479	212.524	-2749.978	-1598.273	92.761
1000	409.237	726.359	473.261	253.098	-2745.239	-1470.576	76.815
1100	415.262	765.651	498.080	294.328	-2741.963	-1343.236	63.785
1200	420.659	802.019	521.912	336.128	-2737.297	-1216.322	52.945
1300	425.513	835.884	544.776	378.441	-2729.077	-1089.907	43.793
1400	429.906	867.580	565.714	421.214	-2720.794	-964.127	35.972
1500	434.090	897.385	587.775	464.415	-2712.461	-838.943	29.215
1600	438.065	925.528	608.013	508.025	-2704.089	-714.314	23.320
1700	441.830	952.199	627.482	552.020	-2697.589	-590.172	18.134
1800	445.554	977.550	646.232	596.391	-2689.835	-466.432	13.536
1900	449.069	1001.744	664.311	641.121	-2710.265	-341.717	9.394
2000	452.625	1024.868	681.765	686.206	-2702.965	-217.244	5.674

Iron Oxide, Magnetite (Fe₃O₄)   CRYSTAL M_r = 231.5386

$S°$(298.15 K) = 145.266 J·K⁻¹·mol⁻¹ $\Delta_f H°$(0 K) = -1114.58 ± 0.8 kJ·mol⁻¹
T_{fus} = 1870 ± 2 K $\Delta_f H°$(298.15 K) = -1120.89 ± 0.8 kJ·mol⁻¹
$\Delta_{fus}H°$ = 138.070 ± 8.4 kJ·mol⁻¹

Enthalpy of Formation

The equilibrium constants for the following four reactions, i.e. (A) $3Fe(cr) + 4H_2O(g) = Fe_3O_4(cr) + 4H_2(g)$; (B) $Fe_3O_4(cr) + H_2(g) = 3FeO(cr) + H_2O(g)$; (C) $Fe_3O_4(cr) + CO(g) = 3FeO(cr) + CO_2(g)$, and (D) $2Fe_3O_4(cr) = 6FeO(cr) + O_2(g)$, have been studied by several investigators. Using their reported equilibrium data, the corresponding enthalpy changes, $\Delta_r H°$(298.15 K), were evaluated by both 2nd and 3rd law methods. Based on the 3rd law value for $\Delta_r H°$(298.15 K), the respective $\Delta_f H°$(298.15 K) values for Fe₃O₄(cr) were also derived. The results obtained are presented as follows.

Source	Reactions	T/K	$\Delta_r H°$(298.15 K), kcal·mol⁻¹ 2nd law	3rd law	$\Delta_f H°$(298.15 K) kcal·mol⁻¹
Fricke, et al.[1]	A	633.2–823.2	-29.68 ± 1.30	-36.91	-268.10
Eastman[2]	B	873.2–1273.2	22.41 ± 0.09	19.29	-268.01
Eastman and Evans[3]	B	973.2–1073.2	21.56 ± 0.07	18.54	-267.26
Emmett and Shultz[4]	B	973.2–1073.2	—	19.18	-267.90
Eastman[2]	C	873.2–1273.2	11.87 ± 0.03	9.38	-267.93
Eastman and Evans[3]	C	973.2–1273.2	11.63 ± 0.03	9.38	-267.94
Salmon[5]	D	1473.2–1673.2	—	153.73	-267.79

The enthalpy change of the reaction $Fe_{0.947}O(cr) + 0.8215\,Fe(cr) + 0.6787\,O_2(g) = 0.5895\,Fe_3O_4(cr)$ has been determined by Humphrey et al.[6] Based on $\Delta_r H°$(298.15 K) = -93.45 kcal·mol⁻¹ (average of two separate values derived from two experimental determinations) and $\Delta_f H°$(wustite, cr, 298.15 K) = -63.64 kcal·mol⁻¹, the value $\Delta_f H°$(Fe₃O₄, cr, 298.15 K) was calculated as -266.5 kcal·mol⁻¹. The enthalpy change, $\Delta_r H°$(298.15 K) = 4.33 kcal·mol⁻¹, for the reaction $3Fe(cr) + 4CO_2(g) = Fe_3O_4(cr) + 4CO(g)$ was reported by Darken and Gurry.[7] The corresponding $\Delta_f H°$(Fe₃O₄, cr, 298.15 K) was evaluated as -266.22 kcal·mol⁻¹. The adopted value of $\Delta_f H°$(298.15 K) for Fe₃O₄(cr) is selected as -267.9 ± 0.2 kcal·mol⁻¹.

Heat Capacity and Entropy

The low temperature heat capacities (60.5–299.7 K) were reported by Millar.[8] The high temperature heat capacities (298–1800 K) were obtained from Coughlin et al.[9] These two sets of data were plotted and joined smoothly at 298.15 K. The $C°_p$ values above 1800 K were obtained by graphical extrapolation. Heat capacities (90–295 K) for Fe₃O₄(cr) were also reported by Parks and Kelley.[10] $S°$(Fe₃O₄, cr, 298.15 K) was derived from the smoothed $C°_p$ data mentioned previously, using $S°$(44.7 K) = 0.969 cal·K⁻¹·mol⁻¹. Coughlin et al.[9] measured the heat-content for magnetite and found a magnetic anomaly around 880 K, corresponding to a maximum in heat capacity. A maximum heat capacity of 37.1 cal·K⁻¹·mol⁻¹ at 114.15 K was also reported by Millar.[8]

Fusion Data

T_{fus} and $\Delta_{fus}H°$ were obtained from Darken and Gurry.[7]

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Iron Oxide, Magnetite (Fe₃O₄)   Fe₃O₄(cr)

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

T/K	$C°_p$	$S°$	$-(G°-H°(T_r))/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹·mol⁻¹			kJ·mol⁻¹			
0	0.	0	INFINITE	-24.571	-1114.579	-1114.579	INFINITE
100	56.335	27.611	254.203	-22.659	-1119.743	-1086.024	567.281
114.150	155.535	37.694	226.660	-21.570	C, LAMBDA MAXIMUM TRANSITION		
114.150	155.279	37.698	226.660	-21.570	C, LAMBDA MAXIMUM TRANSITION		
200	116.945	92.367	157.872	-13.101	-1121.314	-1051.624	274.656
298.15	147.235	145.266	145.266	0.	-1120.894	-1017.438	178.251
300	147.695	146.179	145.269	0.273	-1120.869	-1016.797	177.040
400	171.126	191.952	151.352	16.240	-1118.728	-982.386	128.286
500	192.380	232.441	163.593	34.424	-1115.219	-948.681	99.108
600	212.547	269.299	178.181	54.671	-1110.550	-915.794	79.727
700	232.714	303.578	193.672	76.934	-1104.774	-883.776	65.948
800	252.881	335.969	209.452	101.214	-1098.011	-852.657	55.673
900	273.050	366.919	225.241	127.510	-1090.611	-822.428	47.732
900.000	273.050	366.919	225.241	127.511	C, LAMBDA MAXIMUM TRANSITION		
900.000	273.050	366.919	225.241	127.511	C, LAMBDA MAXIMUM TRANSITION		
1000	200.832	388.079	240.485	147.594	-1091.694	-792.602	41.401
1100	200.832	407.220	254.786	167.677	-1095.556	-762.463	36.206
1200	200.832	424.695	268.228	187.760	-1097.841	-732.139	31.869
1300	200.832	440.770	280.890	207.843	-1095.254	-701.771	28.197
1400	200.832	455.653	292.848	227.927	-1092.980	-671.590	25.057
1500	200.832	469.509	304.169	248.010	-1091.011	-641.562	22.341
1600	200.832	482.471	314.912	268.093	-1089.346	-611.654	19.968
1700	200.832	494.646	325.131	288.176	-1090.831	-581.785	17.876
1800	200.832	506.125	334.870	308.259	-1090.769	-551.846	16.014
1900	200.832	516.984	344.172	328.343	-1133.299	-519.794	14.290
2000	200.832	527.285	353.072	348.426	-1134.548	-487.472	12.731
2100	200.832	537.084	361.603	368.509	-1135.843	-455.087	11.320
2200	200.832	546.426	369.793	388.592	-1137.183	-422.637	10.035
2300	200.832	555.354	377.669	408.675	-1138.568	-390.128	8.860
2400	200.832	563.901	385.252	428.759	-1139.998	-357.557	7.782
2500	200.832	572.099	392.563	448.842	-1141.472	-324.925	6.789
2600	200.832	579.976	399.620	468.925	-1142.988	-292.234	5.871
2700	200.832	587.556	406.441	489.008	-1144.547	-259.482	5.020
2800	200.832	594.859	413.041	509.091	-1146.146	-226.673	4.229
2900	200.832	601.907	419.433	529.175	-1147.786	-193.807	3.491
3000	200.832	608.715	425.629	549.258	-1149.464	-160.882	2.801

Continuation of discussions of selected Fe species

Iron

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