REFERENCE STATE

0	to	2054	K	crystal, alpha
2054	to	2500	K	crystal, beta
2500	to	4963.793	K	liquid
4963.793	to	6000	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°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−5.842	0	0.	0.
100	20.580	17.753	−65.394	−4.764	0.	0.	0
200	24.418	33.561	−45.871	−2.462	0.	0.	0.
298.15	25.687	43.560	43.560	0.	0.	0.	0.
300	25.708	43 719	43.560	0.048	0.	0	0.
400	26.751	51.261	44.581	2.672	0.	0.	0.
500	27.692	57.332	46.543	5.394	0.	0.	0.
600	28.583	62.460	48.780	8.208	0	0.	0
700	29.445	66.932	51.060	11.110	0	0.	0.
800	30.288	70.919	53.298	14.097	0	0.	0.
900	31.120	74.534	55.459	17 167	0.	0.	0.
1000	31.943	77.856	57.535	20.320	0.	0.	0.
1100	32.759	80.938	59.524	23.556	0.	0.	0.
1200	33.572	83.824	61.430	26.872	0.	0.	0.
1300	34.372	86.543	63.258	30.270	0.	0.	0
1400	35.064	89 115	65 014	33.741	0	0.	0.
1500	35.765	91.558	66.703	37.283	0.	0	0.
1600	36.466	93.889	68.330	40.894	0.	0.	0.
1700	37.167	96.121	69.899	44.576	0.	0.	0.
1800	37.868	98.265	71.416	48.328	0.	0.	0.
1900	38.569	100.331	72.884	52.149	0.	0.	0
2000	39.269	102.327	74.306	56.041	0	0.	0.
2054.000	39.648	103.378	75.057	58 172	ALPHA <--> BETA TRANSITION		
2054 000	33.959	106.255	75.057	64.080			
2100	34.384	107.011	75.749	65.652	0	0.	0.
2200	35.307	108.632	77.207	69.136	0.	0.	0.
2300	36.231	110.222	78.608	72.713	0.	0.	0.
2400	37.154	111 784	79 957	76.383	0	0.	0
2500	38.077	113.353	81.262	80.228	0.	0	0.
2500 000	38.077	113.353	81.262	80.228	BETA <--> LIQUID TRANSITION		
2500.000	37 656	125.068	81.262	109.516			
2600	37.656	126.545	82.976	113.281	0.	0.	0
2700	37.656	127 966	84.616	117.047	0.	0.	0
2800	37.656	129.336	86.189	120.813	0	0.	0.
2900	37.656	130.657	87.699	124.578	0.	0.	0.
3000	37.656	131.934	89.153	128.344	0.	0	0.
3100	37.656	133.169	90.553	132.109	0.	0.	0
3200	37.656	134.364	91.903	135.875	0.	0.	0
3300	37.656	135.523	93.208	139 641	0.	0.	0.
3400	37.656	136.647	94.469	143.406	0.	0	0.
3500	37.656	137.739	95.690	147.172	0.	0.	0.
3600	37 656	138.799	96.872	150.937	0	0.	0.
3700	37.656	139.831	98.020	154.703	0	0.	0.
3800	37.656	140.835	99.133	158 469	0.	0.	0.
3900	37.656	141.814	100.215	162.234	0.	0.	0.
4000	37.656	142.767	101.267	166.000	0	0.	0.
4100	37.656	143.697	102.291	169.765	0.	0.	0
4200	37.656	144.604	103.287	173.531	0	0.	0
4300	37.656	145.490	104.258	177.297	0.	0.	0.
4400	37.656	146.356	105.205	181.062	0.	0.	0.
4500	37.656	147.202	106.129	184.828	0	0.	0.
4600	37.656	148.030	107.031	188.593	0.	0.	0
4700	37.656	148.840	107.912	192.359	0.	0.	0.
4800	37.656	149.632	108.773	196.125	0.	0.	0.
4900	37.656	150.409	109.615	199.890	0.	0.	0.
4963.793	37.656	150.896	110.142	202.292	LIQUID <--> IDEAL GAS FUGACITY = 1 bar		
4963 793	37.996	263.754	110.142	762 496			
5000	38.154	264 031	111.256	763.875	0.	0.	0.
5200	39.044	265.544	117.161	771.594	0	0.	0
5400	39.964	267.035	122.684	779.494	0.	0	0.
5600	40 910	268.505	127.866	787.581	0.	0	0.
5800	41.879	269 958	132 741	795.859	0.	0.	0.
6000	42.870	271.394	137.339	804.334	0.	0.	0.

PREVIOUS March 1979 (1 atm) CURRENT March 1979 (1 bar)

$S°(298.15\ K) = 43.560\ J·K^{-1}·mol^{-1}$
$T_{tr} = 2054 \pm 50\ K\ (\alpha–\beta)\ K$

$\Delta_f H°(0\ K) = 0\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ·mol^{-1}$
$\Delta_{tr} H° = 5\,908 \pm 0.2\ kJ·mol^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The adopted thermal functions for α–Hf(cr) are derived from the studies of Collings and Ho,[1] Westrum,[2] Hawkins *et al* [3] and Cezairliyan and McClure.[4] The mathematical and graphical treatment of these four studies yields a continuous and smooth heat capacity curve.

Roberts[5] surveyed the superconductive properties of the elements and reported a critical temperature of 0.128 K for α–Hf(cr). Since this temperature is so low, the effects of superconductivity on the thermal functions are not considered.

There are four studies[1,6–8] on the heat capacty of hafnium in the region 1–5 K. Only Wolcott[6] reported the experimental data (56 data points). In the other three states, an equation (with two constants) was given to describe the entire set of experimental data. The second set of constants given by Betterton and Scarbrough[8] are stated to be an average of the two studies of Kneip *et al.*[7] and the more recent study by Betterton and Scarbrough.[8] However, the values appear suspect and may contain a typographical error. Nevertheless the maximum difference in the calculated values for $S°(5\ K)$ is 0 00024 cal $K^{-1}·mol^{-1}$ with the adopted value being $S°(5\ K) = 0\ 0038\ cal·K^{-1}·mol^{-1}$. Similarly for $C_p°(5\ K)$ the maximum difference is 0.00024 cal $K^{-1}·mol^{-1}$, with the adopted value being $C_p°(5\ K) = 0\ 00638\ cal·K^{-1}·mol^{-1}$

In the region above 5 K, and below 350 K, there are four heat capacity studied.[2,9–11] Cristescu and Simon[9] studies Hf from 13 to 210 K and reported 15 heat capacity values with a peak near 75 K. Burk and Darnell[10] made heat capacity measurements (40–190 K) and reported that the peak is completely absent. The heat capacity measurements of Burk *et al* (10–200 K),[11] and Westrum (5 82–348.55 K)[1,12] support this latter conclusion, i.e., no peak. The values of Burk *et al.*,[11] after correction for the ~2% Zr in this sample, agree with the data of Westrum[2,12] between 10 and 40 K but deviate above 40 K, becoming ~5% higher at 100 K and decreasing to ~1% higher at 200 K. Above 350 K, there are four heat capacity studies and four enthalpy studies.

	Source (Year)	Data Points	T/K	Wt % Zr in Hf Sample
Enthalpy	Adenstedt (1952)[13]	1	373	0.7
	Fieldhouse and Lang (1961)[14]	14	534–1884	1.0
	Hawkins *et al.* (1963)[3]	50	338–1346	2.8
	Golutvin and Maslennikova (1970)[15]	12	551–1309	0.79
	Golutvin and Maslennikova (1970)[15]	9	695–137	0.79
Heat Capacity	Peletskii *et al.* (1971)[16]	13 (smoothed)	1200–2200	0.66
	Arutyunov *et al* (1972)[17]	16 (smoothed)	1100–2050	0.65
	Cezairliyand and McClure (1975)[4]	26	1500–2400	3.12
	Rumyantsev *et al.* (1979)[18]	graph	1000–1900	-

The enthalpy studies show an unusually large scatter within each study as well as a lack of agreement between the studies. The heat capacity studies all have a similar temperature dependence in comparison with the adopted values. However, the studies of Arutyunov *et al.*[17,19] and Rumyantsev *et al.*[18] lie roughly 10% higher than the adopted values, whereas the study of Peletskii *et al.*[16] lies 5–24% below The studies by Arutyunov *et al.*[17,19] and Rumyantsev *et al.*[18] suggest a sharp decrease in the heat capacity values within 50 K of the α–β transition temperature. The experimental results were corrected for this zirconium content.

Transition Data

Refer to the β–crystal table for details.

Sublimation Data

There are no sublimation studies involving α–Hf(cr) The enthalpy of sublimation is calculated as the difference between the enthalpy of formation of the ideal gas and the enthalpy of formation of α–Hf(cr).

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−5.842	0.	0.	0.
100	20.580	17.753	−65.394	−4.764	0.	0.	0.
200	24.418	33.561	−45.871	−2.462	0.	0.	0.
250	25.110	39.086	−43.979	−1.223	0.	0.	0.
298.15	25 687	43.560	43.560	0.	0.	0.	0.
300	25.708	43.719	43.560	0.048	0.	0	0.
350	26.247	47.723	43.875	1.347	0.	0.	0.
400	26.751	51.261	44.581	2.672	0.	0.	0.
450	27.230	54.439	45.503	4.021	0.	0.	0.
500	27 692	57.332	46.543	5.394	0.	0.	0.
600	28.583	62.460	48.780	8.208	0.	0.	0.
700	29 445	66.932	51.060	11.110	0.	0.	0.
800	30.288	70.919	53.298	14.097	0.	0.	0.
900	31.120	74.534	55.459	17.167	0.	0.	0.
1000	31 943	77.856	57.535	20.320	0.	0.	0.
1100	32.759	80.938	59.524	23.556	0.	0	0.
1200	33.572	83.824	61.430	26.872	0.	0	0.
1300	34.372	86.543	63.258	30.270	0.	0.	0.
1400	35.064	89.115	65.014	33.741	0.	0.	0.
1500	35.765	91.558	66.703	37.283	0.	0.	0.
1600	36.466	93.889	68.330	40.894	0.	0.	0.
1700	37.167	96.121	69.899	44.576	0.	0.	0.
1800	37.868	98.265	71.416	48.328	0.	0.	0.
1900	38.569	100.331	72.884	52.149	0.	0.	0.
2000	39.269	102.327	74.306	56.041	0.	0.	0.
2054 000	39 648	103.378	75.057	58.172	---- ALPHA <--> BETA ----		
2100	39.970	104.260	75.687	60.003	−5.648	0.129	−0.003
2200	40.671	106.136	77.029	64.035	−5.101	0.392	−0.009
2300	41.372	107.959	78.334	68.138	−4.576	0.629	−0.014
2400	42.073	109.734	79.605	72.310	−4.073	0.845	−0.018
2500	42 774	111.466	80.845	76.552	−3.676	1 042	−0 022

PREVIOUS CURRENT March 1979

$S°(298.15\ K)$ = [61.104] $J·K^{-1}·mol^{-1}$
T_{trs} = 2054 ± 50 K (α–β) $J·K^{-1}$
T_{fus} = 2500 ± 20 K (β–l) $J·K^{-1}$

$\Delta_f H°(298.15\ K)$ = [18.686] $kJ·mol^{-1}$
$\Delta_{trs}H°$ = 5.908 ± 0.2 $kJ·mol^{-1}$
$\Delta_{fus}H°$ = [29.288 ± 4.2] $kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of formation is calculated from that of the α–crystal by addition of $\Delta_{trs}H°$ and the difference in enthalpy, $H°(2054\ K)–H°(298.15\ K)$, between the α–crsytal and β–crystal.

Heat Capacity and Entropy

The only heat capacity study for the β–crystal is that of Cezairliyand McClure.[1] Using a pulse heating technique, they studied the heat capacity of a sample containing 3.12% (wt) Zr in the range 2054 to 2400 K. These results were corrected by Cezairliyan and McClure[1] to represent pure β–Hf and are extrapolated linearly to the melting point, 2500 K, and to 298.15 K. The entropy at 298.15 is calculated in a manner similar to that for the enthalpy of formation.

Phase Data

Hafnium, at ambient pressures, exists in two crystal modifications. The low temperature form, α–Hf, is hexagonal close packed, an hcp(A3) structure isotypic with Mg. The high temperature form, β–Hf, is body centered cubic, a bcc(A2) structure isotypic with W. The wide variation in the observed transition temperature is undoubtedly due to the effects of various impurities, in particular, zirconium.

Transition Data

Cezairlivan and McClure[2] have summarized the reported transition temperatures for the α to β transition of hafnium. Their summary is given below. All temperatures were corrected to IPTS–68. The pure hafnium value reported by the cited author was corrected for the zirconium content of the alloy. Hultgren *et al.*,[18] based on data available through 1965, recommended T_{trs} = 2013 ± 20 K. We adopt T_{trs} = 2054 ± 50 K based on the study of Cezairliyan and McClure[2] since we have also adopted their measured heat capacity values. In addition there are many studies of binary phase diagrams which lend support to this adopted value.

Source	Zirconium Content (W/%)	Transformation Temperature (K) Hafnium Alloy	Pure Hafnium
Duwez[3] unknown	1586 ± 10		
Fast (1952)[4]	3	1960–2075	
Gibson *et al.* (1958)[5]	0.01	2011	
Deardorff and Kato (1959)[6]	1.2–8.8		2026 ± 20
Peterson and Beernsten (1960)[7]	0.03	1966–2096	
Giessen *et al.* (1963)[8]	2.3	1991 ± 15	2031 ± 20
Ross and Hume–Rothery (1963)[9]	1.6	2236–2266 50	2271 ± 70
Krikorian and Wallace (1964)[10]	0.02–3.45	2007–2100	2016 ± 14
Taylor and Doyle (1964)[11]	2.3	2226 ± 50	2270 ± 70
Romans *et al.* (1965)[12]	1.5	2028	2053
Bates and Barnes (1967)[13]	3.6	2033	
Peletskii and Druzhinin (1971)[14]	0.66	1970 ± 5	
Carlson *et al.* (1973)[15]	3.3	1990–2003	
Cezairliyan and McClure (1976)[2]	3.12	2012 ± 10	2054

Cezairliyand and McClure,[2] using a millisecond–resolution pulse–heating technique, measured the transformation enthalpy to be 33.1 $J·g^{-1}$ (1.412 ± 0.05 $kcal·mol^{-1}$). Peletskii and Druzhinin[14] measured 29 J g^{-1} (1.237 $kcal·mol^{-1}$), a value which is roughly 12% lower than that of Cezairliyan and McClure.[2] Martynyuk and Tsapkov,[16] using a continuous–pulse heating technique, measured a transformation enthalpy of 1.24 $kcal·mol^{-1}$. The samples used in all three studies contained significant amounts of zirconium wt %,[2] 0.66 wt %,[14] and 0.7 wt %,[16] respectively. Hoerster *et al.*[17] measured an enthalpy of transition of 0.52 $kcal·mol^{-1}$ at 2090 K. We adopted $\Delta_{trs}H°$ = 1.412 ± 0.05 $kcal·mol^{-1}$ as derived from the study of Cezairliyan and McClure.[2]

Fusion Data

Refer to the liquid table.

Sublimation Data

The sublimation studies for β–Hf(cr) are summarized on the Hf(g) table The enthalpy of sublimation for Hf(β,cr) is calculated as the difference in the enthalpies of formation at 298.15 K of Hf(g) and Hf(β,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							
100							
200							
250							
298.15	17.747	61.104	61.104	0.	18.686	13.455	−2.357
300	17.764	61.214	61.105	0.033	18.671	13.422	−2.337
350	18.226	63.987	61.323	0.933	18.272	12.579	−1.877
400	18.687	66.451	61.812	1.855	17.869	11.793	−1.540
450	19.149	68.679	62.454	2.801	17.466	11.058	−1.284
500	19.611	70.720	63.180	3.770	17.062	10.368	−1.083
600	20.534	74.377	64.748	5.778	16.255	9.105	−0.793
700	21.457	77.612	66.359	7.877	15.453	7.976	−0.595
800	22.381	80.538	67.951	10.069	14.658	6.963	−0.455
900	23.304	83.227	69.501	12.353	13.872	6.048	−0.351
1000	24.227	85.730	71.000	14.730	13.095	5.221	−0.273
1100	25.151	88.082	72.447	17.199	12.329	4.470	−0.212
1200	26.074	90.310	73.844	19.760	11.573	3.789	−0.165
1300	26.997	92.434	75.193	22.414	10.829	3.171	−0.127
1400	27.921	94.468	76.497	25.160	10.104	2.609	−0.097
1500	28.844	96.426	77.761	27.998	9.401	2.098	−0.073
1600	29.767	98.317	78.987	30.928	8.720	1.634	−0.053
1700	30.691	100.150	80.178	33.951	8.061	1.211	−0.037
1800	31.614	101.930	81.338	37.067	7.424	0.827	−0.024
1900	32.537	103.664	82.467	40.274	6.810	0.477	−0.013
2000	33.461	105.356	83.569	43.574	6.218	0.159	−0.004
2054.000	33.959	106.255	84.154	45.394	---- ALPHA <--> BETA ----		
2100	34.384	107.011	84.646	46.966	0.	0.	0.
2200	35.307	108.632	85.700	50.451	0.	0.	0.
2300	36.231	110.222	86.732	54.028	0.	0.	0.
2400	37.154	111.784	87.743	57.697	0.	0.	0.
2500	38.077	113.353	88.736	61.542	0.	0.	0.
2500.000	38.077	113.353	88.736	61.542	---- BETA <--> LIQUID ----		
2600	39.001	114.865	89.712	65.396	−29.200	1.170	−0.024
2700	39.924	116.354	90.672	69.342	−29.019	2.335	−0.045
2800	40.847	117.822	91.615	73.381	−28.746	3.492	−0.065
2900	41.771	119.272	92.544	77.512	−28.381	4.637	−0.084
3000	42.694	120.704	93.459	81.735	−27.923	5.768	−0.100

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Continued on page 1371

$S°(298.15\ K) = [71.938]\ J·K^{-1}·mol^{-1}$
$T_{fus} = 2500 \pm 20\ K$

$\Delta_f H°(298.15\ K) = [46.209]\ kJ·mol^{-1}$
$\Delta_{fus}H° = [29.288 \pm 4.2]\ kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of formation is calculated from that of the β–crystal by addition of $\Delta_{fus}H°$ and the difference in enthalpy, $H°(2500\ K)–H°(298.15\ K)$, between the β–crystal and liquid.

Heat Capacity and Entropy

There are no heat capacity or enthalpy studies covering the liquid region of hafnium. A constant value of $C_p°$ = 9 0 cal·K^{-1} mol^{-1} is assumed for the region 1820–5500 K. A glass transition is assumed at 1820 K below which extrapolated β–Hf heat capacity values are used. The entropy is calculated in a manner similar to that used for the enthalpy of formation.

Fusion Data

Garg and Ackermann,[1] using pyrometric techniques, measured the melting point of hafnium as 2501 ± 3 K. Hultgren *et al.*[2] reviewed nine studies available through 1955 and recommended T_{fus} = 2500 ± 20 K. We adopted T_{fus} = 2500 ± 20 K.

The studies (and the reported melting temperatures in K) examined by Hultgren *et al.*[2] are: DeBoer and Fast,[3] 2503 ± 50; Skinner *et al.*,[4] 2498; Litton,[5] 2403; Adenstedt,[6] 2248; Spedding,[7] 2508 ± 5; Deardoff and Hayes,[8] (2495 ± 20; Gregorovitch,[9] 2116; Taylor *et al.*,[10] 2503 ± 20.

Ackermann and Rauh[11] measured a melting point of 2467 ± 4 K in a HfO_2 container. However, they state that the melting point may be as high as 2495 K since their sample contained 0.7 wt % Zr.

The enthalpy melting for Hf has not been measured. Various estimates and calculations have been made. Martynyuk *et al* [12] correlated graphically $\Delta_{fus}S°$ versus T_{fus} for many metals and used the resulting linear relationship to estimate $\Delta_{fus}H°$ = 7.0 kcal·mol^{-1}. We adopt this value Ackermann and Rauh[13] measured vapor pressures over Hf(β,cr) and Hf(l), adjusted the vapor pressures for Hf(β,cr) to match those of Hf(l) at T_{fus}, and derived $\Delta_{fus}H°$ = 6.2 kcal·mol^{-1}.

Vaporization Data

The vaporization studies are summarized on the ideal gas table.

The boiling point is calculated as that temperature for which $\Delta G°$ = 0 for Hf(l)=Hf(g) $\Delta_{vap}H°$ is the corresponding enthalpy change. T_{vap} is the temperature at which the fugacity is one bar. The normal boiling point (p=1 bar) would be a slightly lower temperature.

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

T/K	$C_p°$ (J·K^{-1}mol^{-1})	$S°$ (J·K^{-1}mol^{-1})	$-[G°-H°(T_r)]/T$ (J·K^{-1}mol^{-1})	$H°-H°(T_r)$ (kJ·mol^{-1})	$\Delta_f H°$ (kJ·mol^{-1})	$\Delta_f G°$ (kJ·mol^{-1})	log K_f
0							
100							
200							
250							
298.15	17.747	71.938	71.938	0.	46.209	37.748	−6.613
300	17.764	72.048	71.939	0.033	46.194	37.695	−6.563
350	18.226	74.821	72.157	0.933	45.795	36.311	−5.419
400	18 687	77.285	72.646	1.855	45.393	34 983	−4.568
450	19.149	79.513	73.288	2.801	44.989	33.706	−3.912
500	19.611	81.554	74.014	3.770	44.585	32.474	−3.393
600	20.534	85.211	75.582	5.778	43.778	30.128	−2.623
700	21.457	88.446	77.193	7.877	42.976	27.916	−2.083
800	22.381	91.372	78.785	10.069	42.181	25.819	−1.686
900	23.304	94.061	80.335	12.353	41.395	23.821	−1.383
1000	24.227	96.564	81.834	14.730	40.619	21.910	−1.144
1100	25.151	98.916	83.281	17.199	39.852	20.076	−0.953
1200	26.074	101.144	84.678	19.760	39.097	18.312	−0.797
1300	26.997	103.268	86.027	22.414	38.353	16.610	−0.667
1400	27.921	105.302	87.331	25.160	37.627	14.965	−0.558
1500	28.844	107.260	88.595	27.998	36.924	13.371	−0.466
1600	29.767	109.151	89.821	30.928	36.243	11.823	−0.386
1700	30.691	110.984	91.012	33.951	35.584	10.317	−0.317
1800	31.614	112.764	92.172	37.067	34.948	8.849	−0.257
1820.000	31 799	113.114	92.400	37.701	GLASS <--> LIQUID TRANSITION		
1820.000	37.656	113.114	92.400	37.701			
1900	37.656	114.734	93.306	40.713	34.773	7.406	−0.204
2000	37.656	116.666	94 426	44.479	34.646	5.969	−0.156
2100	37.656	118.503	95.529	48.244	28.802	4.669	−0.116
2200	37 656	120.255	96.614	52.010	29.083	3.513	−0.083
2300	37.656	121.929	97.678	55.776	29.271	2.346	−0.053
2400	37.656	123.531	98.722	59.541	29.368	1.173	−0 026
2500	37.656	125.068	99.746	63.307	29.288	0.	0.
2500 000	37.656	125.068	99 746	66.307	BETA <--> LIQUID		
2600	37.656	126.545	100.748	67.072	0.	0	0
2700	37.656	127.966	101.730	70.838	0.	0.	0.
2800	37.656	129.336	102.692	74.604	0	0.	0.
2900	37.656	130.657	103 633	78.369	0.	0.	0.
3000	37 656	131.934	104.556	82.135	0.	0.	0.
3100	37.656	133.169	105.459	85.900	0.	0.	0
3200	37.656	134.364	106.344	89.666	0.	0.	0
3300	37.656	135.523	107.210	93.432	0.	0.	0.
3400	37.656	136.647	108.060	97 197	0	0.	0.
3500	37.656	137.739	108.892	100.963	0.	0.	0.
3600	37.656	138.799	109.708	104 728	0.	0.	0.
3700	37.656	139.831	110.508	108.494	0.	0	0
3800	37.656	140.835	111.293	112.260	0	0.	0.
3900	37.656	141 814	112.063	116.025	0	0.	0.
4000	37 656	142.767	112.819	119.791	0.	0	0.
4100	37.656	143.697	113.561	123.556	0.	0.	0.
4200	37.656	144.604	114.289	127.322	0.	0	0.
4300	37.656	145.490	115.005	131.088	0.	0.	0
4400	37.656	146.356	115.707	134.853	0	0	0.
4500	37.656	147.202	116.398	138.619	0.	0.	0.
4600	37.656	148.030	117.077	142.384	0.	0.	0.
4700	37.656	148.840	117.744	146.150	0.	0.	0.
4800	37.656	149 632	118.400	149.916	0.	0.	0.
4900	37.656	150.409	119.045	153.681	0.	0.	0.
4963 793	37.656	150.896	119.452	156.083	FUGACITY = 1 bar		
5000	37.656	151 170	119.680	157 447	−560.219	4.086	−0.043
5100	37.656	151 915	120.305	161.212	−560.290	15 373	−0.157
5200	37.656	152.646	120.920	164 978	−560.407	26.662	−0.268
5300	37.656	153.364	121.525	168.744	−560.568	37 953	−0 374
5400	37 656	154 068	122.121	172.509	−560.776	49.248	−0.476
5500	37 656	154.759	122.709	176.275	−561.030	60.547	−0.575

PREVIOUS: CURRENT: March 1979

CRYSTAL(α–β)-LIQUID

0	to	2054 K	crystal, alpha
2054	to	2500 K	crystal, beta
above		2500 K	liquid

Refer to the individual tables for details.

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

	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−5.842	0.	0.	0.
100	20.580	17.753	−65.394	−4.764	0.	0.	0.
200	24.418	33.561	−45.871	−2.462	0.	0.	0.
250	25.110	39.086	−43.979	−1.223	0.	0.	0.
298.15	25.687	43.560	43.560	0.	0.	0.	0.
300	25.708	43.719	43.560	0.048	0.	0.	0.
350	26.247	47.723	43.875	1.347	0.	0.	0.
400	26.751	51.261	44.581	2.672	0.	0.	0.
450	27.230	54.439	45.503	4.021	0.	0.	0.
500	27.692	57.332	46.543	5.394	0.	0.	0.
600	28.583	62.460	48.780	8.208	0.	0.	0.
700	29.445	66.932	51.060	11.110	0.	0.	0.
800	30.288	70.919	53.298	14.097	0.	0.	0.
900	31.120	74.534	55.459	17.167	0.	0.	0.
1000	31.943	77.856	57.535	20.320	0.	0.	0.
1100	32.759	80.938	59.524	23.556	0.	0.	0.
1200	33.572	83.824	61.430	26.872	0.	0.	0.
1300	34.372	86.543	63.258	30.270	0.	0.	0
1400	35.064	89.115	65.014	33.741	0.	0.	0.
1500	35.765	91.558	66.703	37.283	0.	0.	0.
1600	36.466	93.889	68.330	40.894	0.	0.	0.
1700	37.167	96.121	69.899	44.576	0.	0.	0.
1800	37.868	98.265	71.416	48.328	0.	0	0.
1900	38.569	100.331	72.884	52.149	0.	0.	0.
2000	39.269	102.327	74.306	56.041	0.	0.	0.
2054.000	39.648	103.378	75.057	58.172	ALPHA <--> BETA TRANSITION		
2054.000	33.959	106.255	75.057	64.080			
2100	34.384	107.011	75.749	65.652	0.	0.	0.
2200	35.307	108.632	77.207	69.136	0.	0	0.
2300	36.231	110.222	78.608	72.713	0.	0.	0.
2400	37.154	111.784	79.957	76.383	0.	0.	0.
2500	38.077	113.353	81.262	80.228	0.	0.	0.
2500.000	38.077	113.353	81.262	80.228	BETA <--> LIQUID TRANSITION		
2500.000	37.656	125.068	81.262	109.516			
2600	37.656	126.545	82.976	113.281	0.	0.	0.
2700	37.656	127.966	84.616	117.047	0.	0.	0.
2800	37.656	129.336	86.189	120.813	0.	0.	0.
2900	37.656	130.657	87.699	124.578	0.	0.	0.
3000	37.656	131.934	89.153	128.344	0.	0.	0
3100	37.656	133.169	90.553	132.109	0.	0.	0.
3200	37.656	134.364	91.903	135.875	0.	0.	0.
3300	37.656	135.523	93.208	139.641	0.	0.	0.
3400	37.656	136.647	94.469	143.406	0.	0.	0.
3500	37.656	137.739	95.690	147.172	0.	0.	0.
3600	37.656	138.799	96.872	150.937	0.	0.	0.
3700	37.656	139.831	98.020	154.703	0.	0.	0.
3800	37.656	140.835	99.133	158.469	0.	0.	0.
3900	37.656	141.814	100.215	162.234	0.	0.	0.
4000	37.656	142.767	101.267	166.000	0.	0.	0.
4100	37.656	143.697	102.291	169.765	0.	0.	0.
4200	37.656	144.604	103.287	173.531	0.	0.	0.
4300	37.656	145.490	104.258	177.297	0.	0.	0.
4400	37.656	146.356	105.205	181.062	0.	0.	0.
4500	37.656	147.202	106.129	184.828	0.	0.	0.
4600	37.656	148.030	107.031	188.593	0.	0.	0.
4700	37.656	148.840	107.912	192.359	0.	0.	0.
4800	37.656	149.632	108.773	196.125	0.	0	0.
4900	37.656	150.409	109.615	199.890	0.	0.	0.
4963.793	37.656	150.896	110.142	202.292	----- FUGACITY = 1 bar -----		
5000	37.656	151.170	110.438	203.656	−560.219	4.086	−0.043
5100	37.656	151.915	111.244	207.421	−560.290	15.373	−0.157
5200	37.656	152.646	112.034	211.187	−560.407	26.662	−0.268
5300	37.656	153.364	112.807	214.953	−560.568	37.953	−0.374
5400	37.656	154.068	113.564	218.718	−560.776	49.248	−0.476
5500	37.656	154.759	114.307	222.484	−561.030	60.547	−0.575

PREVIOUS. CURRENT: March 1979

IP(Hf, g) = 54700 ± 600 cm^{-1}
$S°(298.15\ K)$ = 186.897 ± 0.2 $J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K)$ = 618.0 ± 6.3 $kJ·mol^{-1}$
$\Delta_f H°(298.15\ K)$ = 618.4 ± 6.3 $kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^3F_2$	0.00	5
$^3F_3$	2356.68	7
$^3F_4$	4567.64	9
.	.	.
	53853.61	
IP	54700	

Enthalpy of Formation

There are six sublimation studies and two vaporization studies from which an enthalpy of formation for Hf(g) could be derived. A plot of these vapor pressure data, log p vs $1/T$, reveals considerable discrepancy between the various studies. In the liquid region, the vapor pressure values of Koch *et al* [1] and Ackermann and Rauh[2] are in close agreement. The pressures of the former study are 5% higher at 2500 K but become 10% lower at 2800 K. The measured temperatures in the former study[1] were adjusted (i.e., the pyrometer reading) by Koch *et al.*[1] so that at the observed melting point the temperature would be 2500 K. The sample purity was not stated. In the latter study[2] the reported vapor pressures were corrected pressures (assuming ideal solution) from a eutectic of Hf and W. The Hf sample had a measured melting point of 2464 K; the purity was not reported.

The sublimation studies of Golubtsov and Mikul'skaya[3] and Ackermann and Rauh[2] spanned a temperature range which involved the α- and β-phases of hafnium, yet neither study mentioned the characterization of the condensed phase. The study of Golubtsov and Mikul'skaya[3] is not considered further since their reported vapor pressure equation is ambiguous and cannot be easily modified to yield reasonable vapor pressures. In general terms, the sublimation pressures of Ackermann and Rauh,[2] Kibler *et al.*[4] and McClaine and Blackburn[5] are in reasonable agreement. The pressures of Panish and Reif[6] are 60% above these three studies,[2,4,5] there is considerable scatter with one distinctly low pressure point at 2113 K. On the other hand, the results of Trulson *et al.*[7] are substantially lower by 50% than the three studies[2,4,5] with two distinctly lower points.

A 2nd and 3rd law analysis is given in the following table We adopt $\Delta_f H°$ (Hf, g, 298.15 K) = 147.8 ± 1.5 $kcal·mol^{-1}$. This result is based on the reasonable consistency of the two vapor pressure studies[2,4] with each other and with our adopted thermodynamic functions as evidenced by the small values of the drift. Hultgren *et al.*,[8] using different thermodynamic functions and data available through 1966, recommended an enthalpy of formation of 148.0 ± 1.0 $kcal·mol^{-1}$ based heavily on the study by Kibler *et al.*[4] Other values for $\Delta_f H°(298.15\ K)$, also derived from vapor pressure studies, have been reported by Krupka,[9] Krikorian[10] and Kibler *et al.*[11]

Source (Year)	Reaction*	Pts	T/K	Method	$\Delta_r H°(298.15\ K)$, $kcal·mol^{-1}$ 2nd law	3rd law	Drift $cal·K^{-1}·mol^{-1}$	$\Delta_f H°(298.15\ K)$ $kcal·mol^{-1}$
Kibler *et al.* (1963)[11]	A	8	2035–2325	Langmuir	141.5 ± 2.4	143.4 ± 0.5	0.9 ± 1.1	147.8
Panish and Reif (1963)[6]	A	6	2066–2274	Langmuir	160.3 ± 15.5	140.9 ± 2.7	−9.0 ± 7.2	145.4
McClaine (1964)[6]	A	5	2200–2363	Langmuir	124.3 ± 5.7	144.5 ± 1.3	8.8 ± 2.5	149.0
Trulson *et al.* (1965)[7]	A	15[b]	2075–2273	Knudsen	145.1 ± 4.2	145.9 ± 0.7	0.4 ± 1.9	150.4
Ackermann and Rauh (1972)[2]	A	eqn	1950–2464	mass eff.	145.4	143.6	−0.8	148.0
Koch *et al.* (1968)[1]	B	17	2500–2810	Langmuir	131.6 ± 3.4	136.9 ± 1.2	2.0 ± 1.3	147.9
Ackermann and Rauh (1972)[2]	B	eqn	1464–2800	mass eff.	140.1	136.7	−1.3	147.8

*Reaction. A) Hf(β,cr) = Hf(g) B) Hf(l) = Hf(g) [b]Two points discarded due to a statistical test.

Heat Capacity and Entropy

The electronic energy levels are given in the compilation by Meggers and Moore.[12] Although we have listed only the ground state, the lowest two excited states, the highest observed excited state (below the ionization potential), and the ionization potential for Hf(g), all levels listed by Meggers and Moore,[12] as well as estimated levels (for n = 5,6,7), are used in the calculation. The 233 observed levels, two of which lie above the ionization potential, are too numerous to list completely. In our calculations, the missing levels for n = 6 and 7 have been arbitrarily added near the ionization limit. The calculations indicate that for Hf(g) the thermodynamic functions up to at least 3000 K are independent of the estimated missing levels (for n = 6 and 7), the cut–off procedure, and the inclusion of n = 7 levels. At this temperature there are no experimental heat capacity enthalpy, or vapor pressure data. The Gibbs energy function is essentially unaffected up to 5500 K.

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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	−6.198	618.040	618.040	INFINITE
100	20.786	164.188	205.380	−4.119	619.040	604.397	−315.704
200	20.786	178.596	188.799	−2.041	618.816	589.809	−154.042
250	20.789	183.235	187.240	−1.001	618.617	582.580	−121.723
298.15	20.803	186.897	186.897	0.	618.395	575.659	−100.853
300	20.804	187.026	186.898	0.038	618.386	575.394	−100.185
350	20.854	190.236	187.151	1.080	618.128	568.249	−84.806
400	20.960	193.027	187.715	2.125	617.848	561.142	−73.278
450	21.140	195.505	188.445	3.177	617.551	554.071	−64.315
500	21.397	197.745	189.265	4.240	617.241	547.034	−57.148
600	22.113	201.706	191.017	6.414	616.600	533.053	−46.406
700	23.012	205.181	192.797	8.669	615.954	519.180	−38.742
800	23.991	208.317	194.544	11.019	615.317	505.398	−32.999
900	24.978	211.200	196.236	13.467	614.695	491.696	−28.537
1000	25.925	213.881	197.868	16.013	614.088	478.062	−24.971
1100	26.806	216.394	199.439	18.650	613.490	464.489	−22.057
1200	27.603	218.761	200.952	21.371	612.894	450.969	−19.630
1300	28.305	220.999	202.409	24.167	612.293	437.500	−17.579
1400	28.912	223.119	203.813	27.029	611.683	424.077	−15.823
1500	29.424	225.132	205.168	29.947	611.059	410.698	−14.302
1600	29.847	227.045	206.476	32.911	610.412	397.362	−12.973
1700	30.190	228.865	207.740	35.913	609.733	384.067	−11.801
1800	30.465	230.599	208.962	38.947	609.014	370.813	−10.761
1900	30.681	232.252	210.144	42.004	608.250	357.600	−9.831
2000	30.852	233.830	211.290	45.081	607.435	344.429	−8.996
2100	30.986	235.339	212.399	48.174	600.917	331.429	−8.244
2200	31.095	236.783	213.475	51.278	600.537	318.605	−7.565
2300	31.187	238.167	214.519	54.392	600.074	305.800	−6.945
2400	31.270	239.496	215.532	57.515	599.528	293.017	−6.377
2500	31.351	240.775	216.516	60.646	598.813	280.260	−5.856
2600	31.436	242.006	217.473	63.785	568.899	268.702	−5.398
2700	31.528	243.194	218.404	66.933	568.282	257.168	−4.975
2800	31.632	244.342	219.310	70.091	567.674	245.656	−4.583
2900	31.750	245.454	220.192	73.260	567.077	234.166	−4.218
3000	31.884	246.533	221.052	76.442	566.493	222.696	−3.877
3100	32.037	247.581	221.891	79.638	565.924	211.246	−3.559
3200	32.208	248.601	222.710	82.850	565.370	199.814	−3.262
3300	32.399	249.595	223.510	86.080	564.835	188.398	−2.982
3400	32.610	250.565	224.291	89.330	564.319	176.999	−2.719
3500	32.841	251.513	225.056	92.603	563.826	165.614	−2.472
3600	33.090	252.442	225.803	95.899	563.357	154.243	−2.238
3700	33.359	253.352	226.536	99.221	562.914	142.885	−2.017
3800	33.645	254.246	227.253	102.571	562.498	131.539	−1.808
3900	33.948	255.124	227.957	105.951	562.112	120.203	−1.610
4000	34.267	255.987	228.647	109.362	561.757	108.877	−1.422
4100	34.602	256.837	229.324	112.805	561.435	97.559	−1.243
4200	34.951	257.675	229.989	116.282	561.147	86.248	−1.073
4300	35.313	258.502	230.642	119.796	560.894	74.944	−0.910
4400	35.688	259.318	231.285	123.345	560.678	63.645	−0.756
4500	36.074	260.124	231.917	126.933	560.501	52.351	−0.608
4600	36.471	260.921	232.539	130.561	560.362	41.061	−0.466
4700	36.878	261.710	233.151	134.228	560.264	29.773	−0.331
4800	37.294	262.491	233.754	137.936	560.207	18.486	−0.201
4900	37.720	263.264	234.348	141.687	560.192	7.201	−0.077
4963.793	37.996	263.754	234.723	144.102	----- FUGACITY = 1 bar -----		
5000	38.154	264.031	234.934	145.481	0.	0.	0.
5100	38.595	264.790	235.512	149.318	0.	0.	0.
5200	39.044	265.544	236.083	153.200	0.	0.	0.
5300	39.501	266.292	236.646	157.127	0.	0.	0.
5400	39.964	267.035	237.202	161.100	0.	0.	0.
5500	40.434	267.773	237.751	165.120	0.	0.	0.
5600	40.910	268.505	238.293	169.187	0.	0.	0.
5700	41.392	269.234	238.830	173.302	0	0.	0.
5800	41.879	269.958	239.360	177.465	0.	0.	0.
5900	42.372	270.678	239.885	181.678	0.	0.	0.
6000	42.870	271.394	240.404	185.940	0	0.	0.

PREVIOUS March 1979 (1 atm) CURRENT March 1979 (1 bar)

IP(Hf⁺, g) = 120000 ± 1000 cm⁻¹
$S°$(298.15 K) = 185.040 ± 0.01 J·K⁻¹·mol⁻¹

$\Delta_f H°$(0 K) = 1272.4 ± 4.0 kJ·mol⁻¹
$\Delta_f H°$(298.15 K) = [1278 950] kJ·mol⁻¹

Electronic Levels and Quantum Weights		
State	ϵ_i, cm⁻¹	g_i
$^2D_{3/2}$	0.00	4
$^2D_{5/2}$	3050.88	6
.	.	.
.	.	.
.	.	.
	83129.8	10
IP	120000	

Enthalpy of Formation

$\Delta_f H°$(Hf⁺, g 0 K) is calculated from $\Delta_f H°$(Hf, g, 0 K)[1] using the spectroscopic value of IP(Hf) = 54700 ± 600 cm⁻¹ (654.358 ± 1.18 kJ·mol⁻¹) from Meggers and Moore.[2] The ionization limit is converted from cm⁻¹ to kJ·mol⁻¹ using the factor, 1 cm⁻¹ = 0.01196266 kJ·cm⁻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.

$\Delta_f H°$(Hf⁺, g, 298.15 K) is calculated from $\Delta_f H°$(Hf, g, 0 K) by using IP (Hf) with JANAF[1] enthalpies, $H°(0\ K) - H°(298.15\ K)$, for Hf(g), Hf⁺(g), and e⁻(g). $\Delta_f H°$(Hf → Hf⁺ + 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 electronic energy levels are given in the compilation by Moore.[6] Although we have listed only the ground state, the first excited state, the highest observed excited state, and the ionization potential for Hf⁺(g), all levels listed by Moore,[6] as well as estimated levels (for n = 6 and 7), are used in the calculation. The 121 observed levels are too numerous to list completely. In our calculations the missing levels for n = 6 and 7 have been arbitrarily added near the ionization limit. The calculations indicate that for Hf⁺(g) the thermodyanmic functions up to 5000 K are independent of the estimated missing levels (for n = 6 and 7), the cut-off procedure, and the inclusion of n=7 levels. The free energy function is unaffected up to 10000 K. The reported uncertainty in $S°_{298}$ is due to uncertainties in the gram formula weight and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the higher excited states (n>7), more precise estimation of the missing levels (for all n), and utilization of proper fill and cut-off procedures.[7]

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

T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.		INFINITE	−6.197	1272.397		
100	20.786	162.333	203.521	−4.119			
200	20.786	176.741	186.942	−2.040			
250	20.786	181.379	185.382	−1.001			
298.15	20.786	185.040	185.040	0.	1278.950	1230.512	−215.581
300	20.786	185.169	185.041	0.038	1278.979	1230.212	−214.199
350	20.786	188.373	185.294	1.078	1279.758	1222.022	−182.377
400	20.786	191.149	185.856	2.117	1280.512	1213.722	−158.496
450	20.786	193.597	186.583	3.156	1281.241	1205.329	−139.911
500	20.786	195.787	187.396	4.196	1281.946	1196.857	−125.035
600	20.786	199.577	189.120	6.274	1283.290	1179.711	−102.703
700	20.786	202.781	190.848	8.353	1284.545	1162.347	−86.735
800	20.786	205.556	192.517	10.431	1285.716	1144.810	−74.748
900	20.786	208.005	194.105	12.510	1286.802	1127.130	−65.417
1000	20.786	210.195	195.606	14.589	1287.806	1109.334	−57.946
1100	20.787	212.176	197.024	16.667	1288.729	1091.442	−51.828
1200	20.789	213.985	198.363	18.746	1289.569	1073.469	−46.727
1300	20.794	215.649	199.629	20.825	1290.329	1055.429	−42.408
1400	20.804	217.190	200.829	22.905	1291.016	1037.334	−38.703
1500	20.823	218.626	201.968	24.986	1291.635	1019.192	−35.491
1600	20.857	219.971	203.052	27.070	1292.186	1001.010	−32.680
1700	20.910	221.237	204.085	29.158	1292.671	982.797	−30.198
1800	20.991	222.434	205.071	31.253	1293.092	964.556	−27.991
1900	21.107	223.572	206.015	33.358	1293.454	946.294	−26.015
2000	21.264	224.658	206.920	35.476	1293.759	928.015	−24.237
2100	21.472	225.701	207.790	37.612	1288.363	909.850	−22.631
2200	21.737	226.705	208.627	39.772	1289.117	891.808	−21.174
2300	22.065	227.679	209.434	41.962	1289.808	873.733	−19.843
2400	22.462	228.626	210.214	44.187	1290.444	855.629	−18.622
2500	22.931	229.552	210.970	46.456	1290.946	837.501	−17.499
2600	23.477	230.462	211.702	48.776	1262.291	820.523	−16.485
2700	24.100	231.359	212.413	51.154	1262.982	803.519	−15.545
2800	24.800	232.248	213.106	53.599	1263.739	786.488	−14.672
2900	25.576	233.132	213.781	56.117	1264.571	769.429	−13.859
3000	26.424	234.013	214.441	58.716	1265.483	752.340	−13.099
3100	27.341	234.894	215.086	61.404	1266.484	735.219	−12.388
3200	28.320	235.778	215.719	64.187	1267.579	718.064	−11.721
3300	29.355	236.665	216.340	67.070	1268.776	700.873	−11.094
3400	30.437	237.557	216.951	70.059	1270.078	683.645	−10.503
3500	31.559	238.455	217.553	73.159	1271.490	666.376	−9.945
3600	32.711	239.360	218.146	76.372	1273.017	649.066	−9.418
3700	33.883	240.273	218.732	79.702	1274.659	631.712	−8.918
3800	35.066	241.192	219.311	83.149	1276.420	614.312	−8.444
3900	36.249	242.118	219.884	86.715	1278.298	596.863	−7.994
4000	37.424	243.051	220.451	90.399	1280.295	579.366	−7.566
4100	38.580	243.989	221 014	94.199	1282.409	561.816	−7.158
4200	39.710	244.932	221.572	98.114	1284.636	544.214	−6.768
4300	40.805	245.880	222.126	102.140	1286.975	526.558	−6.396
4400	41.857	246.830	222.677	106.273	1289 422	508.846	−6.041
4500	42.862	247.782	223.224	110.510	1291.971	491.077	−5.700
4600	43.812	248.734	223.768	114.844	1294.618	473.250	−5.374
4700	44.704	249.686	224.310	119.270	1297.358	455.365	−5.061
4800	45.534	250.636	224.848	123.783	1300.183	437.420	−4.760
4900	46.299	251.583	225.384	128.375	1303.088	419.416	−4.471
5000	46.999	252.526	225.918	133.040	745.848	405.438	−4.236
5100	47.631	253.463	226.449	137.772	748.821	398.601	−4.083
5200	48.197	254.393	226.977	142.564	751.810	391.704	−3.935
5300	48.696	255.316	227.503	147.409	754.807	384.751	−3.792
5400	49.130	256.231	228.027	152.301	757.804	377.740	−3.654
5500	49.501	257.136	228.548	157.233	760.795	370 675	−3.520
5600	49.811	258.030	229.066	162.199	763.772	363.555	−3.391
5700	50.063	258.914	229.582	167.194	766 730	356.382	−3.266
5800	50.260	259.787	230.095	172.210	769.662	349.157	−3.144
5900	50.405	260.647	230.606	177.244	772.562	341.882	−3.027
6000	50.502	261.495	231.114	182.290	775.424	334.558	−2.913

PREVIOUS: March 1979 (1 atm) CURRENT: March 1984 (1 bar)

EA(Hf, g) = 0 0 eV
$S°(298.15\ K) = 185.040 \pm 0.002\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 618.040 \pm 6.3\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = [612.197]\ kJ·mol^{-1}$

Electonic Level and Quantum Weight		
State	ϵ_i, cm^{-1}	g_i
$^4F_{3/2}$	0.0	4

Enthalpy of Formation

$\Delta_f H°(Hf^-, g, 0\ K)$ is calculated from $\Delta_f H°(Hf, g, 0\ K)$[1] using the adopted electron affinity of EA(Hf) = −0 0 eV. This value, recommended by Hotop and Lineberger,[2] is based on a semiempirical extrapolation.[3,4] Additional information on $Hf^-(g)$ and may be obtained in the critical discussions of Hotop and Lineberger,[2,4] Rosenstock *et al.*[5] and Massey.[6]

$\Delta_f H°(Hf^-, g, 298.15\ K)$ is obtained from $\Delta_f H°(Hf, g, 0\ K)$ by using EA(Hf) with JANAF[1] enthalpies, $H°(0\ K)–H°(298\ 15\ K)$, for $Hf^-(g)$, Hf(g), and e^-(ref). $\Delta_r H°(Hf^- \rightarrow Hf + e^-, 298.15\ K)$ differs from a room-temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[5] $\Delta_f H°(298.15\ K)$ 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 ground state electronic configuration for $Hf^-(g)$ is given by Hotop and Lineberger[2,4] and Rosenstock *et al.*[5] Lacking any experimental evidence as to the stability of any excited states, we assume that no stable excited states exist.

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

	$J·K^{-1}·mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−6.197	618.040		
100	20.786	162.333	203.521	−4.119			
200	20.786	176.741	186.942	−2.040			
250	20.786	181.379	185.383	−1.001			
298.15	20.786	185.040	185.040	0.	612.197	576.270	−100.960
300	20.786	185.169	185.041	0.038	612.150	576.047	−100.299
350	20.786	188.373	185.294	1.078	610.851	570.132	−85.088
400	20.786	191.149	185.856	2.117	609.526	564.405	−73.704
450	20.786	193.597	186.583	3.156	608.176	558.846	−64.869
500	20.786	195.787	187.396	4.196	606.803	553.438	−57.817
600	20.786	199.577	189.120	6.274	603.989	543.028	−47.275
700	20.786	202.781	190.848	8.353	601 087	533.096	−39.780
800	20.786	205.556	192.517	10.431	598.101	523.586	−34.187
900	20.786	208.005	194.105	12.510	595.030	514.455	−29.858
1000	20.786	210.195	195.606	14.589	591.877	505.671	−26.414
1100	20.786	212.176	197.024	16.667	588.642	497.206	−23.610
1200	20.786	213.984	198.363	18.746	585.325	489 040	−21.287
1300	20.786	215.648	199.629	20.824	581.928	481.153	−19.333
1400	20.786	217.189	200.829	22.903	578.456	473.531	−17.668
1500	20.786	218.623	201.968	24.982	574.915	466.159	−16.233
1600	20.786	219.964	203.052	27.060	571.303	459.026	−14.986
1700	20.786	221.224	204 084	29.139	567.621	452.121	−13.892
1800	20.786	222.412	205.069	31.217	563.870	445.435	−12.926
1900	20.786	223.536	206.012	33.296	560.048	438.959	−12.068
2000	20.786	224 602	206.915	35.375	556.156	432.687	−11.301
2100	20.786	225.617	207.782	37.453	546.546	426.740	−10.615
2200	20.786	226.584	208.615	39.532	543 061	421.116	−9.999
2300	20.786	227.508	209 416	41.610	539 484	415.653	−9.440
2400	20 786	228.392	210.188	43.689	535.815	410.347	−8.931
2500	20.786	229.241	210.934	45.768	531.970	405.198	−8.466
2600	20.786	230.056	211.654	47.846	498.916	401.373	−8.064
2700	20.786	230.840	212.350	49.925	495.150	397.693	−7.694
2800	20.786	231.596	213.024	52.004	491.385	394.153	−7.353
2900	20.786	232.326	213.677	54.082	487 619	390.747	−7.038
3000	20.786	233 030	214.310	56.161	483.854	387.470	−6.746
3100	20 786	233.712	214.925	58.239	480.088	384.320	−6.476
3200	20.786	234.372	215.523	60.318	476.322	381.290	−6.224
3300	20.786	235.012	216.104	62.397	472.557	378.379	−5.989
3400	20.786	235.632	216.669	64.475	468.791	375.581	−5.770
3500	20.786	236.235	217.219	66.554	465.026	372.895	−5.565
3600	20.786	236.820	217.756	68.632	461.260	370.316	−5.373
3700	20 786	237.390	218.279	70 711	457.494	367.841	−5 193
3800	20 786	237.944	218.789	72.790	453.729	365.469	−5.024
3900	20.786	238.484	219.287	74.868	449.963	363.195	−4.864
4000	20.786	239.010	219 774	76.947	446.198	361 018	−4.714
4100	20 786	239.524	220.249	79.025	442.432	358.936	−4.573
4200	20.786	240 024	220.714	81.104	438.666	356.945	−4 439
4300	20 786	240.514	221.169	83.183	434.901	355.043	−4.313
4400	20.786	240.991	221.614	85.261	431.135	353.230	−4.193
4500	20.786	241.459	222.050	87.340	427.370	351.501	−4.080
4600	20.786	241.915	222.477	89.418	423.604	349.857	−3.973
4700	20.786	242.362	222.895	91.497	419 838	348.294	−3.871
4800	20.786	242.800	223.305	93.576	416.073	346.812	−3.774
4900	20.786	243.229	223.707	95.654	412.307	345.408	−3.682
5000	20.786	243.649	224.102	97.733	−151.677	348.167	−3.637
5100	20.786	244 060	224.489	99.811	−155.514	358.202	−3.669
5200	20.786	244.464	224.870	101.890	−159.396	368.313	−3 700
5300	20.786	244.860	225.243	103.969	−163.324	378.499	−3.730
5400	20.786	245.248	225.610	106.047	−167.297	388 759	−3.760
5500	20.786	245.630	225.970	108.126	−171.317	399.093	−3 790
5600	20.786	246.004	226.325	110.204	−175.384	409.501	−3.820
5700	20.786	246.372	226 673	112.283	−179.499	419.982	−3.849
5800	20 786	246.734	227.016	114.362	−183.662	430.535	−3.877
5900	20 786	247.089	227.353	116.440	−187.874	441.161	−3 906
6000	20.786	247.438	227.685	118.519	−192.136	451.858	−3 934

PREVIOUS: March 1979 (1 atm) CURRENT: March 1984 (1 bar)

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REFERENCE STATE

0	to	234.29	K crystal
234.29	to	629.839	K liquid
above		629.839	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°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−9.343	0.	0.	0.
100	24.255	37.219	113.592	−7.637	0.	0.	0.
200	27.275	55.022	80.284	−5.052	0.	0.	0.
234.290	28.485	59.428	76.915	−4.097	CRYSTAL <--> LIQUID TRANSITION		
234.290	28.476	69.225	76.915	−1.802			
298.15	27.978	76.028	76.028	0.	0.	0.	0.
300	27.963	76.201	76.028	0.052	0.	0.	0.
400	27.414	84.161	77.118	2.817	0.	0.	0.
500	27.175	90.248	79.158	5.545	0.	0.	0.
600	27.139	95.197	81.432	8.259	0.	0.	0.
629.839	27.164	96.514	82.115	9.069	LIQUID <--> IDEAL GAS FUGACITY = 1 bar		
629.839	20.786	190.515	82.115	68.274			
700	20.786	192.710	93.092	69.733	0.	0.	0.
800	20.786	195.486	105.722	71.811	0.	0.	0.
900	20.786	197.934	115.834	73.890	0.	0.	0.
1000	20.786	200.124	124.156	75.969	0.	0.	0.
1100	20.786	202.105	131.153	78.047	0.	0.	0.
1200	20.786	203.914	137.143	80.126	0.	0.	0.
1300	20.786	205.578	142.344	82.204	0.	0.	0.
1400	20.786	207.118	146.916	84.283	0.	0.	0.
1500	20.786	208.552	150.978	86.362	0.	0.	0.
1600	20.786	209.894	154.619	88.440	0.	0.	0.
1700	20.786	211.154	157.908	90.519	0.	0.	0.
1800	20.786	212.342	160.899	92.597	0.	0.	0.
1900	20.786	213.466	163.636	94.676	0.	0.	0.
2000	20.786	214.532	166.155	96.755	0.	0.	0.
2100	20.786	215.546	168.483	98.833	0.	0.	0.
2200	20.786	216.513	170.644	100.912	0.	0.	0.
2300	20.786	217.437	172.659	102.990	0.	0.	0.
2400	20.786	218.322	174.543	105.069	0.	0.	0.
2500	20.786	219.170	176.311	107.148	0.	0.	0.
2600	20.786	219.986	177.975	109.226	0.	0.	0.
2700	20.786	220.770	179.546	111.305	0.	0.	0.
2800	20.786	221.526	181.032	113.383	0.	0.	0.
2900	20.786	222.255	182.441	115.462	0.	0.	0.
3000	20.786	222.960	183.780	117.541	0.	0.	0.
3100	20.786	223.642	185.055	119.619	0.	0.	0.
3200	20.786	224.302	186.271	121.698	0.	0.	0.
3300	20.787	224.941	187.433	123.776	0.	0.	0.
3400	20.787	225.562	188.546	125.855	0.	0.	0.
3500	20.787	226.164	189.612	127.934	0.	0.	0.
3600	20.788	226.750	190.635	130.013	0.	0.	0.
3700	20.789	227.319	191.619	132.091	0.	0.	0.
3800	20.790	227.874	192.566	134.170	0.	0.	0.
3900	20.791	228.414	193.478	136.249	0.	0.	0.
4000	20.793	228.940	194.358	138.329	0.	0.	0.
4100	20.795	229.454	195.208	140.408	0.	0.	0.
4200	20.798	229.955	196.029	142.488	0.	0.	0.
4300	20.802	230.444	196.824	144.568	0.	0.	0.
4400	20.807	230.923	197.594	146.648	0.	0.	0.
4500	20.813	231.390	198.339	148.729	0.	0.	0.
4600	20.820	231.848	199.063	150.811	0.	0.	0.
4700	20.829	232.296	199.765	152.893	0.	0.	0.
4800	20.839	232.734	200.448	154.977	0.	0.	0.
4900	20.851	233.164	201.111	157.061	0.	0.	0.
5000	20.866	233.586	201.756	159.147	0.	0.	0.
5100	20.882	233.999	202.384	161.234	0.	0.	0.
5200	20.902	234.405	202.996	163.324	0.	0.	0.
5300	20.924	234.803	203.593	165.415	0.	0.	0.
5400	20.949	235.194	204.174	167.508	0.	0.	0.
5500	20.978	235.579	204.742	169.605	0.	0.	0.
5600	21.010	235.957	205.296	171.704	0.	0.	0.
5700	21.046	236.329	205.837	173.807	0.	0.	0.
5800	21.087	236.696	206.366	175.913	0.	0.	0.
5900	21.132	237.057	206.883	178.024	0.	0.	0.
6000	21.182	237.412	207.389	180.140	0.	0.	0.

PREVIOUS: December 1961 (1 atm) CURRENT: December 1961 (1 bar)