REFERENCE STATE

0	to	1135	K	crystal, alpha
1135	to	2125	K	crystal, beta
2125	to	4702.633	K	liquid
4702.633	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	−5.497	0.	0.	0.
100	18.617	14.055	60.166	−4.611	0.	0.	0.
200	23.873	29.050	41.140	−2.418	0.	0.	0.
298.15	25.202	38.869	38.869	0.	0.	0.	0.
300	25.218	39.025	38.870	0.047	0.	0.	0.
400	25.935	46.384	39.868	2.606	0.	0.	0.
500	26.564	52.238	41.776	5.231	0.	0.	0.
600	27.281	57.143	43.939	7.922	0.	0.	0.
700	28.053	61.406	46.136	10.689	0.	0.	0.
800	28.966	65.210	48.287	13.538	0.	0.	0.
900	30.003	68.680	50.363	16.486	0.	0.	0.
1000	31.128	71.899	52.357	19.542	0.	0.	0.
1100	32.306	74.921	54.272	22.713	0.	0.	0.
1135.000	32.724	75.939	54.925	23.851	ALPHA <--> BETA		
1135.000	28.329	79.478	54.925	27.868	TRANSITION		
1200	28.511	81.060	56.298	29.715	0.	0.	0.
1300	28.879	83.356	58.292	32.584	0.	0.	0.
1400	29.353	85.513	60.160	35.494	0.	0.	0.
1500	29.934	87.558	61.919	38.458	0.	0.	0.
1600	30.621	89.511	63.583	41.485	0.	0.	0.
1700	31.414	91.390	65.164	44.585	0.	0.	0.
1800	32.314	93.211	66.672	47.771	0.	0.	0.
1900	33.320	94.985	68.115	51.052	0.	0.	0.
2000	34.433	96.722	69.502	54.439	0.	0.	0.
2100	35.652	98.431	70.839	57.942	0.	0.	0.
2125.000	35.973	98.854	71.166	58.837	BETA <--> LIQUID		
2125.000	41.840	108.699	71.166	79.757	TRANSITION		
2200	41.840	110.150	72.471	82.895	0.	0.	0.
2300	41.840	112.010	74.150	87.079	0.	0.	0.
2400	41.840	113.791	75.765	91.263	0.	0.	0.
2500	41.840	115.499	77.320	95.447	0.	0.	0.
2600	41.840	117.140	78.820	99.631	0.	0.	0.
2700	41.840	118.719	80.269	103.815	0.	0.	0.
2800	41.840	120.241	81.669	107.999	0.	0.	0.
2900	41.840	121.709	83.025	112.183	0.	0.	0.
3000	41.840	123.127	84.338	116.367	0.	0.	0.
3100	41.840	124.499	85.612	120.551	0.	0.	0.
3200	41.840	125.827	86.848	124.735	0.	0.	0.
3300	41.840	127.115	88.049	128.919	0.	0.	0.
3400	41.840	128.364	89.216	133.103	0.	0.	0.
3500	41.840	129.577	90.352	137.287	0.	0.	0.
3600	41.840	130.756	91.458	141.471	0.	0.	0.
3700	41.840	131.902	92.536	145.655	0.	0.	0.
3800	41.840	133.018	93.586	149.839	0.	0.	0.
3900	41.840	134.105	94.611	154.023	0.	0.	0.
4000	41.840	135.164	95.612	158.207	0.	0.	0.
4100	41.840	136.197	96.589	162.391	0.	0.	0.
4200	41.840	137.205	97.544	166.575	0.	0.	0.
4300	41.840	138.190	98.478	170.759	0.	0.	0.
4400	41.840	139.152	99.392	174.943	0.	0.	0.
4500	41.840	140.092	100.286	179.127	0.	0.	0.
4600	41.840	141.011	101.161	183.311	0.	0.	0.
4700	41.840	141.911	102.019	187.495	0.	0.	0.
4702.633	41.840	141.935	102.041	187.605	LIQUID <--> IDEAL GAS		
4702.633	38.083	261.292	102.041	748.899	FUGACITY = 1 bar		
4800	38.268	262.074	105.279	752.616	0.	0.	0.
4900	38.445	262.865	108.487	756.451	0.	0.	0.
5000	38.608	263.643	111.583	760.304	0.	0.	0.
5200	38.894	265.163	117.460	768.055	0.	0.	0.
5400	39.126	266.636	122.958	775.858	0.	0.	0.
5600	39.306	268.062	128.115	783.702	0.	0.	0.
5800	39.437	269.444	132.965	791.577	0.	0.	0.
6000	39.522	270.782	137.537	799.474	0.	0.	0.

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

$S°(298.15\ K) = 38.87 \pm 0.2\ J·K^{-1}·mol^{-1}$
$T_{tr} = 1135 \pm 10\ K\ (\alpha–\beta)$

$\Delta_f H°(0\ K) = 0\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ·mol^{-1}$
$\Delta_{tr} H° = 4.017 \pm 0.3\ kJ·mol^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The adopted thermal functions for α–Zr(cr) are derived from the studies of Collings and Ho,[1] Wolcott,[2] Burk *et al.*,[3] Skinner and Johnston,[4] Todd,[5] and Scott.[6] The mathematical and graphical treatment of these four studies yields a continuous and smooth heat capacity curve.

There are six studies[1,2,7–10] on the heat capacity of zirconium in the region 1–5 K. Only Wolcott[2] reported the experimental data (60 data points). In the other studies, an equation (with two constants) was given to describe the entire set of experimental data. The constants given by Collings and Ho[1] and the data of Wolcott[2] were used in this region. The maximum difference in the calculated values for $S°(5\ K)$ is 0.00029 $cal·mol^{-1}·K^{-1}$, with the adopted value being $S°(5\ K) = 0.0043\ cal·mol^{-1}·K^{-1}$ Similarly for $C_p°(5\ K)$ the maximum difference is 0.00073 $cal·mol^{-1}·K^{-1}$, with the adopted value being $C_p°(5\ K) = 0.00610\ cal·mol^{-1}·K^{-1}$.

In the region above 5 K and below 300 K, there are four heat capacity studies.[2–5] There is much scatter among the different studies, between 150 and 300 K. From 150–200 K, we adopt graphically smoothed C_p values intermediate between Burk *et al.*,[2] Skinner and Johnston,[4] and Todd.[5] From 200–300 K, we adopt the data of Skinner and Johnston,[4] because it meshes better with the high temperature data. Burk's data is 1.4% higher than the adopted at 170 K, Todd's data is 0.7% higher and Skinner's data ia 1% lower. Todd's data is 3% higher than the adopted at 300 K.

Between 300 K and 1135 K there are three heat capacity studies[6,11,12] and seven enthalpy studies.[13–19] The three heat capacity studies show much scatter and disagreement. The data of Scott[6] was adopted, although only the data from runs 17 and 64, out of a total of nine runs, was actually used in the fit. None of Scott's data below 540 K were used in the fit, becuase the data had a hump in this region and appeared to be high. The region between the low temperature data (300 K) and 540 K was graphically smoothed to assure continuity in the C_p curve. The data of Scott[6] is about 5% higher than the adopted between 300 and 540 K. Between 540 and 960 K it is within ±3% of the adopted. From 960 K to the transition temperature, there is much scatter; some of the data are as much as 20% higher than the adopted. The data of Vollmer *et al.*[12] are about 3% lower than the adopted at 300 K. Between 540 and 580 it agrees with the adopted. From 580–1000 K it is about 1.5% higher than the adopted. The data of Klein and Danielson[11] was given only as a graph. It is considerably lower than the adopted values.

The enthalpy studies show an unusually large scatter within each study, as well as a lack of agreement between the studies. When plotted as mean heat capacity, the seven studies are all higher than the adopted values, by 2 to 40%.

Transition Data

Refer to the β–Zr(cr) table for details.

Sublimation Data

There are no experimental sublimation studies involving α–Zr(cr) The enthalpy of sublimation is calculated as the difference between the enthalpy of formation of the monatomic gas and the enthalpy of formation of α–Zr(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	−5.497	0.	0.	0.
100	18.617	14.055	60.166	−4.611	0.	0.	0.
200	23.873	29.050	41.140	−2.418	0.	0.	0.
250	24.693	34.474	39.281	−1.202	0.	0.	0.
298.15	25.202	38.869	38.869	0.	0.	0.	0.
300	25.218	39.025	38.870	0.047	0.	0.	0.
350	25.606	42.943	39.178	1.318	0.	0.	0.
400	25.935	46.384	39.868	2.606	0.	0.	0.
450	26.246	49.457	40.756	3.911	0.	0.	0.
500	26.564	52.238	41.776	5.231	0.	0.	0.
600	27.281	57.143	43.939	7.922	0.	0.	0.
700	28.053	61.406	46.136	10.689	0.	0.	0.
800	28.966	65.210	48.287	13.538	0.	0.	0.
900	30.003	68.680	50.363	16.486	0.	0.	0.
1000	31.128	71.899	52.357	19.542	0.	0.	0.
1100	32.306	74.921	54.272	22.713	0.	0.	0.
1135.000	32.724	75.939	54.925	23.851	---- ALPHA <--> BETA ----		
1200	33.502	77.783	56.113	26.004	−3.711	0.222	−0.010
1300	34.681	80.511	57.886	29.413	−3.170	0.528	−0.021
1400	35.807	83.123	59.596	32.938	−2.556	0.790	−0.029
1500	36.846	85.630	61.249	36.572	−1.886	1.006	−0.035
1600	37.762	88.038	62.848	40.304	−1.181	1.176	−0.038
1700	38.520	90.351	64.398	44.119	−0.466	1.301	−0.040

PREVIOUS. December 1967 CURRENT: June 1979

$S°(298.15\ K)$ = [43.192] $J·K^{-1}·mol^{-1}$
T_{trs} = 1135 ± 10 K (α–β)
T_{fus} = 2125 ± 15 K (β–l)

$\Delta_f H°(298.15\ K)$ = [4.810] $kJ·mol^{-1}$
$\Delta_{trs}H°$ = 4.017 ± 0.3 $kJ·mol^{-1}$
$\Delta_{fus}H°$ = 20.92 ± 6.3 $kJ·mol^{-1}$

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, $H°(1135\ K)–H°(298.15\ K)$, between the α–crystal and the β–crystal.

Heat Capacity and Entropy

There are five heat capacity studies[1–5] and five enthalpy studies[6–10] over the temperature range 1135–2125 K. The adopted values were based on the heat capcity study of Cezairliyan and Righini.[4] The data of Scott[1] showed much scatter with a maximum deviation of 7% from the adopted. The data of Rumyantsu *et al.*[5] were largely scattered and about 15% high. The data of Vollmer *et al.*[3] and of Klein and Danielson[2] were 5–10% lower than the adopted. The enthalpy studies show an unusually large scatter within each study, as well as lack of agreement between the studies. Like the α–Zr(cr), the mean heat capacities are all higher than the adopted values, by 3 to 10%. The entropy at 298.15 K is calculated in a manner similar to that for the enthalpy of formation.

Phase Data

Zirconium, at ambient pressures, exists in two crystal modifications. The low temperature form, α–Zr, is hexagonal close packed, an hcp (A3) structure isotypic with Mg. The high temperature form, β–Zr, is body centered cubic, a bcc (A2) structure.

Transition Data

The transition temperature and enthalpies of transition are summarized in the table below. The adopted value of T_{trs} is 1135 ± 10 K. The adopted $\Delta_{trs}H°$ is 4.017 $kJ·mol^{-1}$.

Source	T_{trs}/K	$\Delta_{trs}H°$, $kcal·mol^{-1}$	Purity	Method
Vogel and Tonn[11]	1135 ± 5	–	–	cooling and dilatometric curves
Jaeger and Veenstra[12]	<1150	–	–	drop calorimetry
Coughlin and King[6]	1135	0.920	97.85	drop calorimetry
Dewey[13]	1138 ± 10	–	–	cooling curve
Skinner[7]	1143 ± 5	1.042	99.05	drop calorimetry
Komar and Shrednik[14]	1135	–	–	electron microscope
Scott[1]	1143 ± 2	0.993 ± 0.025	–	adiabatic calorimetry
Douglas and Victor[9]	1136	0.894	99.91	drop calorimetry
Gertzricken and Slyusar[15]	1135	0.712 ± 0.060	–	differential calorimetry
Klein and Danielson[2]	1138	–	–	resistivity
Rudy *et al.*[16]	1145 ± 15	–	99.81	differential thermal analysis
Vollmer *et al.*[3]	1155	0.950	99.8	adiabatic calorimetry
Peletskii *et al.*[17]	1148 ± 5	–	–	resistivity
Martynyuk and Tsapkov[18]	–	1.076	99.76	resistivity

Fusion Data

Refer to the liquid table for details.

Sublimation Data

The sublimation studies involving β–Zr(cr) are summarized on the Zr(g) table. The enthalpy of sublimation for β–Zr(cr) is calculated as the difference in the enthalpies of formation at 298.15 K of Zr(g) and β–Zr(cr).

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

T/K	$C_p°$ ($J·K^{-1}·mol^{-1}$)	$S° - [G°-H°(T_r)]/T$ ($J·K^{-1}·mol^{-1}$)	$H°-H°(T_r)$ ($kJ·mol^{-1}$)	$\Delta_f H°$ ($kJ·mol^{-1}$)	$\Delta_f G°$ ($kJ·mol^{-1}$)	log K_f
0						
100						
200						
250						
298.15	25.202	43.192	43.192	0.	4.810	3.521	−0.617
300	25.218	43.348	43.193	0.047	4.810	3.513	−0.612
350	25.587	47.264	43.501	1.317	4.809	3.297	−0.492
400	25.935	50.703	44.191	2.605	4.809	3.081	−0.402
450	26.238	53.775	45.088	3.909	4.808	2.865	−0.333
500	26.564	56.557	46.098	5.229	4.808	2.649	−0.277
600	27.281	61.462	48.261	7.921	4.809	2.217	−0.193
700	28.053	65.724	50.457	10.687	4.808	1.785	−0.133
800	28.966	69.535	52.608	13.542	4.813	1.353	−0.088
900	28.473	72.916	54.681	16.412	4.736	0.923	−0.054
1000	28.238	75.902	56.656	19.245	4.513	0.511	−0.027
1100	28.260	78.592	58.530	22.068	4.164	0.126	−0.006
1135.000	28.329	79.478	59.163	23.058	---- ALPHA <--> BETA ----		
1200	28.511	81.060	60.306	24.905	0.	0.	0.
1300	28.879	83.356	61.992	27.774	0.	0.	0.
1400	29.353	85.513	63.596	30.684	0.	0.	0.
1500	29.934	87.558	65.126	33.648	0.	0.	0.
1600	30.621	89.511	66.589	36.675	0.	0.	0.
1700	31.414	91.390	67.993	39.776	0.	0.	0.
1800	32.314	93.211	69.344	42.961	0.	0.	0.
1900	33.320	94.985	70.647	46.242	0.	0.	0.
2000	34.433	96.722	71.907	49.629	0.	0.	0.
2100	35.652	98.431	73.130	53.132	0.	0.	0.
2125.000	35.973	98.854	73.430	54.027	---- BETA <--> LIQUID ----		
2200	36.977	100.119	74.318	56.763	−21.323	0.746	−0.018
2300	38.409	101.794	75.476	60.531	−21.738	1.759	−0.040
2400	39.947	103.461	76.608	64.448	−22.005	2.786	−0.061
2500	41.591	105.125	77.715	68.524	−22.113	3.822	−0.080
2600	43.342	106.790	78.801	72.770	−22.052	4.859	−0.098

PREVIOUS: December 1967 CURRENT: June 1979

$S°(298.15\ K) = [47.605]\ J·K^{-1}·mol^{-1}$
$T_{fus} = 2125 \pm 15\ K$

$\Delta_f H°(298.15\ K) = [17.404]\ kJ·mol^{-1}$
$\Delta_{fus}H° = 20.92 \pm 6.3\ kJ·mol^{-1}$

Enthalpyof Formation

The enthalpy of formation is calculated from that of the β–crystal by addition of $\Delta_{fus}H°$ and the difference in enthalpy, $H°(2125\ K)–H°(298.15\ K)$, between the β–crystal and the liquid.

Heat Capacity and Entropy

There are no heat capacity or enthalpy studies covering the liquid region of zirconium. A constant value of $C_p° = 41.84\ J·K^{-1}·mol^{-1}$ is assumed for the region 2125–5500 K. A glass transition is assumed at 1580 K below which extrapolated β–Zr heat capacity values are used. The entropy is calculated in a manner similar to that used for the enthalpy of formation.

Fusion Data

The available fusion temperature and enthalpy of fusion data are summarized in the table below. We adopt $T_{fus} = 2125 \pm 15$ K and $\Delta_{fus}H° = 20.92 \pm 6.3\ kJ·mol^{-1}$.

Source	T_{fus}/k	$\Delta_{fus}H°$, kcal·mol^{-1}
deBoer and Fast[1]	2130	
Adenstedt [2]	2113	
Oriani and Jones [3]	2125 ± 2	
Deardorff and Hayes [4]	2128	
Scott [5]	2118	
Klein and Danielson [6]	2118	
Rudy et al [7]	2150 ± 20	
Sara [8]	2133 ± 15	
Rudy and Windisch [9]	2149 ± 4	
Elyutin et al [10]		5.0 ± 0.3
Ackerman and Rauk [11]	2134	
Martynyuk and Tsapkov [12]		5.139

Vaporization Data

The vaporization studies are summarized on the Zr(g) table. The boiling point is calculated as that temperature for which $\Delta_r G° = 0$ for $Zr(l) = Zr(g)$. $\Delta_{vap}H°$ is the corresponding enthalpy change. T_{vap} is the temperature at which the fugacity is one bar.

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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							
100							
200							
250							
298.15	25.202	47.605	47.605	0.	17.404	14.799	−2.593
300	25.218	47.761	47.605	0.047	17.404	14.783	−2.574
350	25.606	51.678	47.914	1.318	17.404	14.346	−2.141
400	25.935	55.120	48.604	2.606	17.404	13.910	−1.816
450	26.246	58.192	49.502	3.911	17.404	13.473	−1.564
500	26.564	60.974	50.512	5.231	17.404	13.036	−1.362
600	27.281	65.878	52.675	7.922	17.404	12.162	−1.059
700	28.053	70.141	54.872	10.689	17.404	11.289	−0.842
800	28.966	73.945	57.022	13.538	17.404	10.415	−0.680
900	30.003	77.416	59.098	16.486	17.404	9.542	−0.554
1000	31.128	80.635	61.093	19.542	17.404	8.668	−0.453
1100	32.306	83.656	63.008	22.713	17.404	7.795	−0.370
1200	33.502	86.519	64.849	26.004	13.693	7.143	−0.311
1300	34.681	89.247	66.622	29.413	14.234	6.575	−0.264
1400	35.807	91.859	68.332	32.938	14.848	5.964	−0.223
1500	36.846	94.365	69.984	36.572	15.518	5.306	−0.185
1580.000	37.614	96.300	71.268	39.551	GLASS <--> LIQUID TRANSITION		
1580.000	41.840	96.300	71.268	39.551			
1600	41.840	96.826	71.584	40.387	16.307	4.602	−0.150
1700	41.840	99.363	73.144	44.571	17.390	3.837	−0.118
1800	41.840	101.754	74.668	48.755	18.388	3.010	−0.087
1900	41.840	104.016	76.154	52.939	19.291	2.131	−0.059
2000	41.840	106.163	77.601	57.123	20.089	1.207	−0.032
2100	41.840	108.204	79.010	61.307	20.769	0.245	−0.006
2125.000	41.840	108.699	79.356	62.353	BETA <--> LIQUID		
2200	41.840	110.150	80.382	65.491	0.	0.	0.
2300	41.840	112.010	81.717	69.675	0.	0.	0.
2400	41.840	113.791	83.016	73.859	0.	0.	0.
2500	41.840	115.499	84.282	78.043	0.	0.	0.
2600	41.840	117.140	85.514	82.227	0.	0.	0.
2700	41.840	118.719	86.715	86.411	0.	0.	0.
2800	41.840	120.241	87.885	90.595	0.	0.	0.
2900	41.840	121.709	89.026	94.779	0.	0.	0.
3000	41.840	123.127	90.139	98.963	0.	0.	0.
3100	41.840	124.499	91.226	103.147	0.	0.	0.
3200	41.840	125.828	92.286	107.331	0.	0.	0.
3300	41.840	127.115	93.322	111.515	0.	0.	0.
3400	41.840	128.364	94.335	115.699	0.	0.	0.
3500	41.840	129.577	95.324	119.883	0.	0	0.
3600	41.840	130.756	96.292	124.067	0.	0.	0.
3700	41.840	131.902	97.239	128.251	0.	0.	0.
3800	41.840	133.018	98.166	132.435	0.	0.	0.
3900	41.840	134.105	99.074	136.619	0.	0.	0.
4000	41.840	135.164	99.963	140.803	0.	0.	0.
4100	41.840	136.197	100.834	144.987	0.	0.	0.
4200	41.840	137.205	101.688	149.171	0.	0.	0.
4300	41.840	138.190	102.526	153.355	0.	0.	0.
4400	41.840	139.152	103.347	157.539	0.	0.	0.
4500	41.840	140.092	104.153	161.723	0.	0.	0.
4600	41.840	141.011	104.945	165.907	0.	0.	0.
4700	41.840	141.911	105.722	170.091	0.	0.	0.
4702.633	41.840	141.935	105.742	170.201	FUGACITY = 1 bar		
4800	41.840	142.792	106.485	174.275	−560.936	11.617	−0.126
4900	41.840	143.655	107.235	178.459	−560.588	23.542	−0.251
5000	41.840	144.500	107.971	182.643	−560.257	35.459	−0.370
5100	41.840	145.329	108.696	186.827	−559.941	47.371	−0.485
5200	41.840	146.141	109.408	191.011	−559.640	59.276	−0.595
5300	41.840	146.938	110.109	195.195	−559.352	71.175	−0.701
5400	41.840	147.720	110.798	199.379	−559.075	83.069	−0.804
5500	41.840	148.488	111.476	203.563	−558.809	94.958	−0.902

PREVIOUS. December 1967 CURRENT: June 1979

CRYSTAL(α-β)-LIQUID

0	to	1135 K	crystal, alpha
1135	to	2125 K	crystal, beta
above		2125 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°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
	J·K⁻¹mol⁻¹			kJ·mol⁻¹			
0	0.	0.	INFINITE	−5.497	0.	0.	0.
100	18.617	14.055	60.166	−4.611	0.	0.	0.
200	23.873	29.050	41.140	−2.418	0.	0.	0.
250	24.693	34.474	39.281	−1.202	0.	0.	0.
298.15	25.202	38.869	38.869	0.	0.	0.	0.
300	25.218	39.025	38.870	0.047	0.	0.	0.
350	25.606	42.943	39.178	1.318	0.	0.	0.
400	25.935	46.384	39.868	2.606	0.	0.	0.
450	26.246	49.457	40.766	3.911	0.	0.	0.
500	26.564	52.238	41.776	5.231	0.	0.	0.
600	27.281	57.143	43.939	7.922	0.	0.	0.
700	28.053	61.406	46.136	10.689	0.	0.	0.
800	28.966	65.210	48.287	13.538	0.	0.	0.
900	30.003	68.680	50.363	16.486	0.	0.	0.
1000	31.128	71.899	52.357	19.542	0.	0.	0.
1100	32.306	74.921	54.272	22.713	0.	0.	0.
1135.000	32.724	75.939	54.925	23.851	ALPHA <--> BETA TRANSITION		
1135.000	28.329	79.478	54.925	27.868			
1200	28.511	81.060	56.298	29.715	0.	0.	0.
1300	28.879	83.356	58.292	32.584	0.	0.	0.
1400	29.353	85.513	60.160	35.494	0.	0.	0.
1500	29.934	87.558	61.919	38.458	0.	0.	0.
1600	30.621	89.511	63.583	41.485	0.	0.	0.
1700	31.414	91.390	65.164	44.585	0.	0.	0.
1800	32.314	93.211	66.672	47.771	0.	0.	0.
1900	33.320	94.985	68.115	51.052	0.	0.	0.
2000	34.433	96.722	69.502	54.439	0.	0.	0.
2100	35.652	98.431	70.839	57.942	0.	0.	0.
2125.000	35.973	98.854	71.166	58.837	BETA <--> LIQUID TRANSITION		
2125.000	41.840	108.699	71.166	79.757			
2200	41.840	110.150	72.471	82.895	0.	0.	0.
2300	41.840	112.010	74.150	87.079	0.	0.	0.
2400	41.840	113.791	75.765	91.263	0.	0.	0.
2500	41.840	115.499	77.320	95.447	0.	0.	0.
2600	41.840	117.140	78.820	99.631	0.	0.	0.
2700	41.840	118.719	80.269	103.815	0.	0.	0.
2800	41.840	120.241	81.669	107.999	0.	0.	0.
2900	41.840	121.709	83.025	112.183	0.	0.	0.
3000	41.840	123.127	84.338	116.367	0.	0.	0.
3100	41.840	124.499	85.612	120.551	0.	0.	0.
3200	41.840	125.827	86.848	124.735	0.	0.	0.
3300	41.840	127.115	88.049	128.919	0.	0.	0.
3400	41.840	128.364	89.216	133.103	0.	0.	0.
3500	41.840	129.577	90.352	137.287	0.	0.	0.
3600	41.840	130.756	91.458	141.471	0.	0.	0.
3700	41.840	131.902	92.536	145.655	0.	0.	0.
3800	41.840	133.018	93.586	149.839	0.	0.	0.
3900	41.840	134.105	94.611	154.023	0.	0.	0.
4000	41.840	135.164	95.612	158.207	0.	0.	0.
4100	41.840	136.197	96.589	162.391	0.	0.	0.
4200	41.840	137.205	97.544	166.575	0.	0.	0.
4300	41.840	138.190	98.478	170.759	0.	0.	0.
4400	41.840	139.152	99.392	174.943	0.	0.	0.
4500	41.840	140.092	100.286	179.127	0.	0.	0.
4600	41.840	141.011	101.161	183.311	0.	0.	0.
4700	41.840	141.911	102.019	187.495	0.	0.	0.
4702.633	41.840	141.935	102.041	187.605	FUGACITY = 1 bar		
4800	41.840	142.792	102.859	191.679	−560.936	11.617	−0.126
4900	41.840	143.655	103.683	195.863	−560.588	23.542	−0.251
5000	41.840	144.500	104.491	200.047	−560.257	35.459	−0.370
5100	41.840	145.329	105.283	204.231	−559.941	47.371	−0.485
5200	41.840	146.141	106.061	208.415	−559.640	59.276	−0.595
5300	41.840	146.938	106.825	212.599	−559.352	71.175	−0.701
5400	41.840	147.720	107.575	216.783	−559.075	83.069	−0.804
5500	41.840	148.488	108.312	220.967	−558.809	94.958	−0.902

PREVIOUS: CURRENT: June 1979

IP(Zr, g) = 55145 ± 500 cm^{-1}
$S°(298.15\ K) = 181.343 \pm 0.04\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 608.7 \pm 8.4\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 610.0 \pm 8.4\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^3F_2$	0.00	5
$^3F_3$	570.41	7
$^3F_4$	1240.84	9
–	–	–
–	–	–
–	–	–
IP_0^1	51899.40	3
IP	55145	

Enthalpy of Formatiom

Vapor pressures over Zr(β) and Zr(l) were measured, using the Langmuir free–vaporization method, by Zwikker,[1] Skinner *et al.*,[2] Fidorov and Smirnov[3,4] and Koch and Anable.[5] Trulson and Goldstein[6] used a mass spectrometric method with a high temperature Knudson effusion source to obtain the vapor pressure for Zr(β) and Zr(l). Similarly, Ackermann and Rauh[7] determined the vapor pressure for Zr(l) by a combination of mass effusion and mass spectrometric techniques. In this latter study the reported values (equation only) were obtained from vapor pressure measurements over Zr(l) saturated with tungsten. These values were then corrected for the dissolved tungsten by the corresponding mole fraction.

A plot of log p vs. 1/T for the above mentioned studies reveals considerable discrepancy. The results of Fredorov and Smirnov[3,4] are an order of magnitude higher than those of Zwikker,[1] however, both studies appear inconsistent with the other studies involving Zr(β).[2,6,7] The sublimation studies of Golubtsov *et al.*[9] and Sumin and Peizularz[10] reported $\Delta_f H°(0\ K)$ values of 143.1 ± 0.22 and 145.6 ± 0.4 $kcal·mol^{-1}$, respectively. The experimental data is not given in either study.

A second and third law evaluation of seven studies yields an adopted enthalpy of formation value, $\Delta_f H°(298.15\ K, Zr, g) = 145.8 \pm 2.0$ $kcal·mol^{-1}$. This adopted value is a weighted average of four vapor pressure studies.[2,5,6,7] Hultgren,[8] using different thermodynamic functions and data available through 1967, recommended a enthalpy of foramtion (at 298.15 K) of 145.5 ± 1.0 $kcal·mol^{-1}$, based primarily on the data of Skinner *et al.*[2]

Investigator	Reaction	T/K	Points	$\Delta_f H°(298.15\ K)$, $kcal·mol^{-1}$ 2nd law	3rd law	Drift $cal·K^{-1}·mol^{-1}$	$\Delta_f H°(298.15\ K)$ $kcal·mol^{-1}$
Zwikker[1]	a	1600–2100	Eqn	62.9	139.6	41.5	140.8
Skinner *et al.*[2]	a	1949–2054	12	144.2 ± 3.0	146.5 ± 0.3	1.2 ± 1.0	147.7
Trulson and Goldstein[6]	a	1968–2112	14	143.0 ± 3.6	142.8 ± 0.5	−0.1 ± 1.8	144.0
Federov *et al.*[3,4]	a	1498–1723	6	59.9 ± 0.1	122.4 ± 6.8	39.0 ± 0.1	123.6
Ackermann and Rauh[7]	a	1975–2100	Eqn	148.5	144.4	−2.0	145.6
Trulson and Goldstein[6]	b	2148–2274	8	129.7 ± 4.9	137.7 ± 0.6	3.6 ± 2.2	142.7
Koch and Anable[5]	b	2229–2795	16	144.5 ± 4.2	144.1 ± 2.4	−0.2 ± 1.7	149.1
Ackermann and Rauh[7]	b	2150–2500	Eqn	139.6	139.3	−0.1	144.3

Reactions: a. Zr(β) = Zr(g) b. Zr(l) = Zr(g)

Heat Capacity and Entropy

The electronic energy levels are given in the compilation by Moore.[11,12] Although we have only listed the ground state, first two excited states, the highest observed excited state, and the ionization limit for Zr(g), all levels listed by Moore,[11,12] as well as estimated missing levels for $n = 5$ and 6, are used in our calculations. The observed levels are too numerous to list completely. Our calculations indicate that for Zr(g) the thermochemical functions are independent of the estimated missing levels for $n = 5$ and 6 (levels estimated and included above 52000 cm^{-1}) and the cut–off procedure up to 4000 K. The Gibbs energy function is essentially unaffected (<0.001 $kcal·mol^{-1}$) up to 6000 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 more exact estimation of excited states for $n = 5$ and 6, the consideration of states for $n > 6$, and the utilization of proper fill and cut–off procedures.[13]

References

[1]C. Zwikker, Versl. Kon. Ak. van Wetenschappen, Amsterdam 35, 336 (1926); Proc. Roy. Ac. Amsterdam 29, 792 (1926); Physica 8, 240 (1928); and J. H. deBoer and J. D. Fack, Z. anorg. allgem. Chem. 187, 193 (1930).

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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	.000	.000	INFINITE	−6.816	608.709	608.709	INFINITE
100	21.000	155.846	203.189	−4.734	609.904	595.725	−311.175
150	22.249	164.561	188.944	−3.657	609.946	588.621	−204.976
200	24.029	171.205	183.708	−2.501	609.944	581.514	−151.876
250	25.576	176.740	181.776	−1.259	609.970	574.404	−120.015
298.15	26.641	181.343	181.343	.000	610.027	567.549	−99.432
300	26.674	181.507	181.343	.049	610.030	567.285	−98.773
350	27.344	185.675	181.671	1.401	610.111	560.155	−83.599
400	27.664	189.350	182.406	2.778	610.199	553.012	−72.216
450	27.718	192.614	183.362	4.163	610.280	545.859	−63.362
500	27.589	195.529	184.436	5.547	610.343	538.697	−56.277
600	27.045	200.514	186.714	8.280	610.385	524.362	−45.650
700	26.424	204.636	188.989	10.953	610.292	510.031	−38.059
800	25.934	208.130	191.168	13.570	610.058	495.722	−32.367
900	25.660	211.167	193.225	16.147	609.689	481.451	−27.943
1000	25.610	213.866	195.157	18.709	609.194	467.227	−24.405
1100	25.754	216.312	196.971	21.276	608.590	453.059	−21.514
1200	26.048	218.565	198.677	23.865	604.177	439.172	−19.117
1300	26.442	220.665	200.289	26.489	603.932	425.431	−17.094
1400	26.895	222.641	201.816	29.155	603.688	411.710	−15.361
1500	27.371	224.513	203.267	31.869	603.438	398.006	−13.860
1600	27.844	226.294	204.651	34.629	603.172	384.319	−12.547
1700	28.298	227.996	205.974	37.437	602.878	370.649	−11.389
1800	28.724	229.626	207.243	40.288	602.544	356.998	−10.360
1900	29.118	231.189	208.463	43.180	602.156	343.367	−9.440
2000	29.482	232.692	209.637	46.111	601.699	329.758	−8.612
2100	29.819	234.139	210.770	49.076	601.161	316.174	−7.864
2200	30.134	235.534	211.864	52.074	579.206	303.363	−7.203
2300	30.432	236.880	212.922	55.102	578.050	290.850	−6.605
2400	30.719	238.181	213.948	58.160	576.924	278.388	−6.059
2500	31.000	239.441	214.942	61.246	575.826	265.971	−5.557
2600	31.279	240.662	215.908	64.360	574.756	253.598	−5.095
2700	31.559	241.848	216.847	67.501	573.713	241.266	−4.668
2800	31.843	243.000	217.761	70.671	572.699	228.972	−4.272
2900	32.132	244.123	218.650	73.870	571.714	216.713	−3.903
3000	32.428	245.217	219.518	77.098	570.758	204.488	−3.560
3100	32.729	246.285	220.364	80.356	569.832	192.295	−3.240
3200	33.037	247.329	221.190	83.644	568.936	180.130	−2.940
3300	33.350	248.351	221.998	86.963	568.071	167.994	−2.659
3400	33.666	249.351	222.788	90.314	567.238	155.883	−2.395
3500	33.985	250.331	223.561	93.697	566.437	143.796	−2.146
3600	34.306	251.293	224.318	97.111	565.667	131.731	−1.911
3700	34.626	252.238	225.060	100.558	564.930	119.688	−1.690
3800	34.944	253.165	225.787	104.036	564.224	107.664	−1.480
3900	35.258	254.077	226.501	107.547	563.551	95.658	−1.281
4000	35.568	254.974	227.202	111.088	562.908	83.669	−1.093
4100	35.871	255.856	227.890	114.660	562.296	71.695	−.913
4200	36.167	256.724	228.566	118.262	561.714	59.737	−.743
4300	36.455	257.578	229.231	121.893	561.161	47.791	−.581
4400	36.733	258.419	229.885	125.552	560.636	35.859	−.426
4500	37.001	259.248	230.528	129.239	560.139	23.938	−.278
4600	37.258	260.064	231.161	132.952	559.668	12.027	−.137
4700	37.488	260.867	231.785	136.685	559.217	.127	−.001
4800	37.717	261.658	232.399	140.446	0.000	.000	.000
4900	37.934	262.438	233.004	144.228	0.000	.000	.000
5000	38.137	263.207	233.600	148.032	0.000	.000	.000
5100	38.327	263.964	234.188	151.855	0.000	.000	.000
5200	38.503	264.710	234.768	155.697	0.000	.000	.000
5300	38.666	265.445	235.340	159.556	0.000	.000	
5400	38.816	266.169	235.904	163.430	0.000	.000	.000
5500	38.952	266.882	236.461	167.318	0.000	.000	.000
5600	39.074	267.585	237.010	171.220	0.000	.000	.000
5700	39.184	268.278	237.553	175.133	0.000	.000	.000
5800	39.281	268.960	238.089	179.056	0.000	.000	.000
5900	39.366	269.633	238.618	182.989	0.000	.000	.000
6000	39.438	270.295	239.140	186.929	0.000	.000	.000

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

$IP(Zr^+, g) = 105900 \pm 100\ cm^{-1}$
$S°(298..15\ K) = 183.639 \pm 0.04\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 1268.4 \pm 25.1\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = [1276.563]\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^4F_{3/2}$	0.00	4
$^4F_{5/2}$	314.67	6
$^4F_{7/2}$	763.44	8
$^4F_{9/2}$	1322.91	10
–	–	–
–	–	–
–	–	–
$^2H_{11/12}$	91737.40	12
IP	105900	

Enthalpy of Formation

$\Delta_f H°(Zr^+, g, 0\ K)$ is calculated from $\Delta_f H°(Zr, g, 0\ K)$[1] using the spectroscopic value of $IP(Zr) = 55145 \pm 5\ cm^{-1}$ ($659.68 \pm 0.06\ kJ·mol^{-1}$) from 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.

$\Delta_f H°(Zr^+, g, 298.15\ K)$ is calculated from $\Delta_f H°(Zr, g, 0\ K)$ by using IP(Zr) with JANAF[1] enthalpies, $H°(0\ K)–H°(298.15\ K)$, for Zr(g), Zr^+(g), and e^-(g). $\Delta_f H°(Zr \rightarrow Zr^+ + e^-, 298.15\ K)$ 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 compilations by Moore.[2,6] Although we have only listed the ground state, first three excited states, the highest observed excited state, and the ionization limit for Zr^+(g), all levels listed by Moore,[2,6] as well as estimated missing levels for $n = 5$ and 6, are used in our calculations. The observed levels are too numerous to list completely. Our calculations indicate that for Zr^+(g) the thermochemical functions are independent of the estimated missing levels for $n = 5$ and 6 (levels estimated and included above 90000 cm^{-1}) and the cut–off procedure up to 6000 K. The Gibbs energy function is essentially unaffected (<0.001 $cal·mol^{-1}·K^{-1}$) up to 12000 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 more exact estimation of excited states for $n = 5$ and 6, the consideration of states for $n>6$, and the utilization of proper fill and cut–off procedures.[7]

References

[1]JANAF Thermochemical Tables: Zr(g), 6–30–79; e^-(g), 3–31–82.
[2]C. E. Moore, U.S. Nat. Bur. Stand., NSRDS–NBS–34, 8 pp. (1970).
[3]E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).
[4]H. M. Rosenstock, K. Draxl, *et al.*, J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).
[5]R. D. Levin and Lias,. U.S. Nat. Bur. Stand., NSRDS–NBS–71, 634 pp. (1982).
[6]C. E. Moore, U.S. Nat. Bur. Stand., NSRS–NBS–35, Volume II, 1970 [Reprint of NBS Circular 467, Volume II, 1952].
[7]J. R. Downey, Jr., The Dow Chemical Company, AFOSR–TR–78–0960, Contract No. F44620–75–1–0048, (1978).

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	.000	.000	INFINITE	−7.472	1268.391		
100	23.495	154.699	208.027	−5.333			
150	26.127	164.776	192.014	−4.086			
200	27.404	172.491	186.207	−2.743			
250	28.010	178.679	184.104	−1.356			
298.15	28.282	183.639	183.639	.000	1276.563	1227.145	−214.991
300	28.288	183.814	183.640	.052	1276.607	1226.838	−213.612
350	28.358	188.182	183.985	1.469	1277.792	1218.450	−181.844
400	28.280	191.965	184.751	2.886	1278.959	1209.892	−157.996
450	28.112	195.287	185.741	4.296	1280.104	1201.190	−139.430
500	27.905	198.238	186.846	5.696	1281.224	1192.361	−124.565
600	27.513	203.290	189.179	8.466	1283.381	1174.384	−102.239
700	27.268	207.510	191.505	11.204	1285.431	1156.054	−86.266
800	27.188	211.145	193.738	13.925	1287.381	1137.438	−74.267
900	27.232	214.348	195.853	16.646	1289.233	1118.583	−64.921
1000	27.351	217.223	197.849	19.374	1290.984	1099.527	−57.433
1100	27.502	219.837	199.731	22.117	1292.634	1080.300	−51.299
1200	27.658	222.237	201.508	24.875	1290.469	1061.150	−46.191
1300	27.803	224.456	203.189	27.648	1292.452	1041.959	−41.866
1400	27.928	226.522	204.782	30.435	1294.407	1022.617	−38.154
1500	28.031	228.452	206.297	33.233	1296.320	1003.137	−34.932
1600	28.110	230.264	207.739	36.040	1298.179	983.530	−32.109
1700	28.169	231.970	209.114	38.854	1299.971	963.809	−29.614
1800	28.208	233.581	210.429	41.673	1301.683	943.985	−27.394
1900	28.233	235.107	211.688	44.495	1303.303	924.069	−25.404
2000	28.244	236.555	212.896	47.319	1304.818	904.069	−23.612
2100	28.245	237.933	214.055	50.144	1306.218	883.997	−21.988
2200	28.238	239.247	215.171	52.968	1286.168	864.606	−20.528
2300	28.225	240.502	216.245	55.791	1286.886	845.428	−19.200
2400	28.208	241.703	217.281	58.613	1287.602	826.219	−17.982
2500	28.187	242.854	218.281	61.433	1288.316	806.980	−16.861
2600	28.164	243.959	219.248	64.250	1289.028	787.713	−15.825
2700	28.139	245.022	220.183	67.066	1289.738	768.418	−14.866
2800	28.114	246.045	221.088	69.878	1290.445	749.097	−13.975
2900	28.087	247.031	221.966	72.688	1291.150	729.750	−13.144
3000	28.060	247.983	222.817	75.496	1291.852	710.380	−12.369
3100	28.033	248.902	223.644	78.300	1292.551	690.986	−11.643
3200	28.006	249.792	224.447	81.102	1293.248	671.569	−10.962
3300	27.979	250.653	225.228	83.902	1293.942	652.131	−10.322
3400	27.951	251.488	225.989	86.698	1294.633	632.672	−9.720
3500	27.924	252.298	226.729	89.492	1295.321	613.192	−9.151
3600	27.897	253.084	227.450	92.283	1296.007	593.693	−8.614
3700	27.869	253.848	228.153	95.071	1296.690	574.175	−8.106
3800	27.842	254.591	228.839	97.857	1297.370	554.639	−7.624
3900	27.816	255.314	229.509	100.640	1298.048	535.084	−7.167
4000	27.789	256.018	230.163	103.420	1298.722	515.513	−6.732
4100	27.763	256.704	230.802	106.197	1299.395	495.924	−6.318
4200	27.737	257.372	231.426	108.972	1300.064	476.319	−5.924
4300	27.712	258.025	232.038	111.745	1300.731	456.698	−5.548
4400	27.687	258.661	232.635	114.515	1301.396	437.062	−5.189
4500	27.664	259.283	233.221	117.282	1302.058	417.410	−4.845
4600	27.641	259.891	233.794	120.048	1302.718	397.744	−4.517
4700	27.619	260.485	234.356	122.811	1303.375	378.064	−4.202
4800	27.599	261.067	234.906	125.571	743.094	369.987	−4.026
4900	27.579	261.636	235.446	128.330	744.096	362.203	−3.861
5000	27.561	262.193	235.975	131.087	745.079	354.399	−3.702
5100	27.545	262.738	236.494	133.843	746.044	346.576	−3.550
5200	27.530	263.273	237.004	136.596	746.994	338.734	−3.403
5300	27.517	263.797	237.505	139.349	747.929	330.874	−3.261
5400	27.505	264.311	237.997	142.100	748.852	322.997	−3.124
5500	27.495	264.816	238.480	144.850	749.763	315.102	−2.993
5600	27.488	265.311	238.954	147.599	750.664	307.191	−2.865
5700	27.481	265.798	239.421	150.347	751.557	299.264	−2.742
5800	27.477	266.276	239.880	153.095	752.442	291.321	−2.624
5900	27.475	266.745	240.331	155.843	753.322	283.363	−2.509

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