REFERENCE STATE

0	to 692.73	K	crystal
692.73	to 1180.173	K	liquid
above	1180.173	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	−5.669	0.	0.	0.
100	19.455	16.523	63.224	−4.670	0.	0.	0.
200	24.050	31.820	44.005	−2.437	0.	0.	0.
298.15	25.387	41.717	41.717	0.	0.	0.	0.
300	25.406	41.874	41.717	0.047	0.	0.	0.
400	26.346	49.314	42.725	2.636	0.	0.	0.
500	27.386	55.301	44.660	5.321	0.	0.	0.
600	28.588	60.399	46.868	8.118	0.	0.	0.
692.730	29.802	64.591	48.965	10.825	CRYSTAL <--> LIQUID TRANSITION		
692.730	31.380	75.161	48.965	18.147			
700	31.380	75.489	49.239	18.375	0.	0.	0.
800	31.380	79.679	52.788	21.513	0.	0.	0.
900	31.380	83.375	55.985	24.651	0.	0.	0.
1000	31.380	86.681	58.892	27.789	0.	0.	0.
1100	31.380	89.672	61.557	30.927	0.	0.	0.
1180.173	31.380	91.880	63.542	33.443	LIQUID <--> IDEAL GAS FUGACITY = 1 bar		
1180.173	20.786	189.586	63.542	148.754			
1200	20.786	189.933	65.628	149.166	0.	0.	0.
1300	20.786	191.597	75.255	151.244	0.	0.	0.
1400	20.786	193.137	83.620	153.323	0.	0.	0.
1500	20.786	194.571	90.970	155.402	0.	0.	0.
1600	20.786	195.913	97.487	157.480	0.	0.	0.
1700	20.786	197.173	103.315	159.559	0.	0.	0.
1800	20.786	198.361	108.562	161.637	0.	0.	0.
1900	20.786	199.485	113.318	163.716	0.	0.	0.
2000	20.786	200.551	117.653	165.795	0.	0.	0.
2100	20.786	201.565	121.625	167.873	0.	0.	0.
2200	20.786	202.532	125.281	169.952	0.	0.	0.
2300	20.786	203.456	128.660	172.030	0.	0.	0.
2400	20.786	204.341	131.795	174.109	0.	0.	0.
2500	20.786	205.189	134.714	176.188	0.	0.	0.
2600	20.786	206.004	137.440	178.266	0.	0.	0.
2700	20.787	206.789	139.994	180.345	0.	0.	0.
2800	20.787	207.545	142.393	182.424	0.	0.	0.
2900	20.788	208.274	144.653	184.502	0.	0.	0.
3000	20.789	208.979	146.785	186.581	0.	0.	0.
3100	20.791	209.661	148.803	188.660	0.	0.	0.
3200	20.793	210.321	150.715	190.739	0.	0.	0.
3300	20.796	210.961	152.531	192.819	0.	0.	0.
3400	20.800	211.582	154.258	194.899	0.	0.	0.
3500	20.806	212.185	155.905	196.979	0.	0.	0.
3600	20.814	212.771	157.476	199.060	0.	0.	0.
3700	20.824	213.341	158.979	201.142	0.	0.	0.
3800	20.836	213.897	160.417	203.225	0.	0.	0.
3900	20.852	214.438	161.795	205.309	0.	0.	0.
4000	20.871	214.966	163.117	207.395	0.	0.	0.
4100	20.894	215.482	164.388	209.483	0.	0.	0.
4200	20.922	215.986	165.611	211.574	0.	0.	0.
4300	20.955	216.478	166.788	213.668	0.	0.	0.
4400	20.994	216.961	167.923	215.765	0.	0.	0.
4500	21.039	217.433	169.018	217.867	0.	0.	0.
4600	21.091	217.896	170.076	219.973	0.	0.	0.
4700	21.150	218.350	171.098	222.085	0.	0.	0.
4800	21.218	218.796	172.087	224.204	0.	0.	0.
4900	21.295	219.234	173.045	226.329	0.	0.	0.
5000	21.381	219.665	173.973	228.463	0.	0.	0.
5100	21.478	220.090	174.873	230.606	0.	0.	0.
5200	21.585	220.508	175.746	232.759	0.	0.	0.
5300	21.703	220.920	176.595	234.923	0.	0.	0.
5400	21.833	221.327	177.420	237.100	0.	0.	0.
5500	21.976	221.729	178.222	239.290	0.	0.	0.
5600	22.131	222.126	179.002	241.496	0.	0.	0.
5700	22.300	222.519	179.762	243.717	0.	0.	0.
5800	22.482	222.909	180.503	245.956	0.	0.	0.
5900	22.680	223.295	181.225	248.214	0.	0.	0.
6000	22.892	223.678	181.929	250.492	0.	0.	0.

PREVIOUS. December 1978 (1 atm) CURRENT: December 1978 (1 bar)

Pearson Notation: hP2
$S°(298.15\ K) = 41.717 \pm 0.17\ J·K^{-1}·mol^{-1}$
$T_{fus} = 692.73\ K$

$\Delta_f H°(0\ K) = 0\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ·mol^{-1}$
$\Delta_{fus} H° = 7.322 \pm 0.105\ kJ·mol^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The adopted heat capacity values are derived from the low temperature heat capacity studies of Martin[1] and Zabetakis[2] and four high temperature enthalpy studies.[3,4,5,6] The heat capacity values at the temperature where these two different types of study join are forced to be smooth and continuous.

The results of Martin[1] differ from the adopted values by less than 1% in the range 14–30 K. The results of Zabetakis[2] also agree within 0.4% in the region 23–195 K. In the region 200–260 K, the data of Zabetakis[2] indicated a slight depression of 0.2 $cal·K^{-1}·mol^{-1}$ at the mid–point of this region. Other low temperature studies did not support this result, so that the adopted heat capacity values are smoothed in this region to be in better agreement with the studies of Behrens and Drucker,[7] Bronson and Wilson,[8] and Eichenauer and Schulze.[9] The enthalpy data of Jaeger and Poppema,[6] Eastman *et al.*,[4] Ruer and Kremers,[5] and Schubel[3] all agree within 1% of the adopted enthalpy vlaues.

The thermodynamic functions are based on $S°(12\ K) = 0.0230\ cal·K^{-1}·mol^{-1}$ and $H°(12\ K)–H°(0\ K) = 0.20\ cal·mol^{-1}$. These values are obtained by integration of smoothed low temperature data and are in agreement with the values used by Martin[1] and Zabetakis.[2] Below 0.850 ± 0.01 K, zinc is a superconductive element; this behavior is summarized in a recent review by Roberts.[10] The literature survey for Zn was done in part by Hultgren,[11] his help is greatly appreciated.

Fusion Data

We adopt $\Delta_{fus}H° = 1.750 \pm 0.025\ kcal·mol^{-1}$. This value is derived primarily from the adiabatic calorimetric study of Chiotti *et al.*[12] Numerous other studies (over 20) reported values in the range 1.504–1.850 $kcal·mol^{-1}$ with a mean of 1.735 $kcal·mol^{-1}$.

The adopted value for $T_{fus} = 692.73$ K is a primary reference point on the IPTS–68.[13]

Sublimation Data

The sublimation studies are summarized on the Zn(g) table.

References

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

	$J·K^{-1}·mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−5.669	0.	0.	0.
100	19.455	16.523	63.224	−4.670	0.	0.	0.
200	24.050	31.820	44.005	−2.437	0.	0.	0.
250	25.039	37.290	42.132	−1.211	0.	0.	0.
298.15	25.387	41.717	41.717	0.	0.	0.	0.
300	25.406	41.874	41.717	0.047	0.	0.	0.
350	25.889	45.828	42.028	1.330	0.	0.	0.
400	26.346	49.314	42.725	2.636	0.	0.	0.
450	26.843	52.446	43.634	3.965	0.	0.	0.
500	27.386	55.301	44.660	5.321	0.	0.	0.
600	28.588	60.399	46.868	8.118	0.	0.	0.
692.730	29.802	64.591	48.965	10.825	--- CRYSTAL <--> LIQUID ---		
700	29.900	64.903	49.129	11.042	−7.333	0.077	−0.006
800	31.284	68.985	51.360	14.101	−7.412	1.143	−0.075
900	32.716	72.752	53.530	17.300	−7.351	2.210	−0.128
1000	34.178	76.275	55.630	20.645	−7.144	3.262	−0.170

PREVIOUS: CURRENT: December 1978

$S°(298.15\ K)$ = [50.792] $J·K^{-1}·mol^{-1}$
T_{fus} = 692.73 K

$\Delta_f H°(298.15\ K)$ = [6.519] $kJ·mol^{-1}$
$\Delta_{fus}H°$ = 7.322 ± 0.105 $kJ·mol^{-1}$

Enthalpy of Formation

The enthalpy of formation of Zn(l) at 298.15 K is calculated from that of the crystal by adding $\Delta_{fus}H°$ and the difference in enthalpy, $H°(692.73\ K)–H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

The adopted heat capacity for Zn(l) is 7.5 $cal·K^{-1}·mol^{-1}$. It is taken as a constant for the real liquid region. There are five enthalpy and two heat capacity studies on liquid zinc. The enthalpy studies are summarized in the following table. The $C_p°$ value given is that derived from the enthalpy data assuming a linear temperature dependence.

Source	Reference Year	Temperature	No. of Observations Liquid	Total	T/K	$C_p°$ (l) $cal·K^{-1}·mol^{-1}$
[1]	1919	293	28	47	469–992	8.14
[2]	1920	293	15	18	675–1140	7.24
[3]	1926	273	6	14	323–1123	8.20
[4]	1926	291	4	9	483–914	6.69
[5]	1960	471	2	13	481–723	7.0

Forster and Tschentke[6] reported heat capacity data graphically in the region 723–973 K. Their study showed a heat capacity of approximately 8.2 $cal·K^{-1}·mol^{-1}$ at the melting point with a steadily decreasing trend to 7.0 $cal·K^{-1}·mol^{-1}$ at 973 K. Cordoba[7] measured heat capacities in the crystal and liquid region, including 22 experimental points in the liquid region up to 798.2 K. This study resulted in a parabolic temperature dependence, with a minimum at 730 K of $C_p°$ = 6.8 $cal·K^{-1}·mol^{-1}$ and rapidly increasing values on either side of this minimum.

All these heat capacity and enthalpy studies do not conclusively define the temperature dependence of the heat capacity of liquid zinc. In addition, some of these heat capacity and enthalpy studies[3,4,7] do not show good agreement with the adopted values in the crystal region. However, the adopted constant value is consistent with the experimental data (within the uncertainty of the data) and with the vaporization data. The literature survey for Zn was done in part by Hultgren.[8]

Fusion Data

Refer to the crystal table for details.

Vaporization Data

There are numerous studies on the vaporization of liquid zinc.[2,9–22] These studies, when depicted graphically in a log p vs 1/T plot, show remarkably good agreement in the region T_{fus} to 1666 K (approximately 0.2 to 23000 mmHg) with the exception of the studies by Ruff and Bergdahl[10] and Piacente *et al.*[22] A 2nd and 3rd law analysis of all zinc vaporization studies up to 400 mmHg is summarized in the following table.

Source	Year	Number Observations	Method	Vaporization Studies T/K	Drift $cal·mol^{-1}·K^{-1}$	$\Delta_{vap}H°(298.15\ K)$, $kcal·mol^{-1}$ 2nd law	3rd law
[9]	1919	7	boiling point	926–1198	−1.3 ± 1.0	31.91 ± 1.02	30.58 ± 0.40
[10]	1920	5	transport	761–995	−0.1 ± 0.1	29.67 ± 0.10	29.62 ± 0.04
[11]	1925	30	boiling point	857–960	−0.4 ± 0.1	29.94 ± 0.07	29.61 ± 0.04
[12]	1926	21	static	903–1259	−0.6 ± 0.1	30.22 ± 0.14	29.58 ± 0.10
[14]	1934	1	transport	954			29.68
[15]	1934	6	static	955–1089	0.6 ± 0.7	28.90 ± 0.66	29.52 ± 0.16
[16]	1955	eqn	torsion effusion	700–900	0.0	29.60	29.60
[17]	1957	3	transport	862–1020	−0.2 ± 0.1	29.76 ± 0.05	29.62 ± 0.02
[18]	1959	3	transport	823–923	0.6 ± 0.1	29.08 ± 0.04	29.62 ± 0.06
[22]	1973	10	transpiration	826–1041	−0.1 ± 0.3	29.94 ± 0.25	29.86 ± 0.11

Not including the results of Ruff and Bergdahl[10] and Piacente *et al.*,[22] the mean of the tabulated 3rd law values is $\Delta_{vap}H°(298.15\ K)$ = 29.59 ± 0.1 $kcal·mol^{-1}$. This may be compared with our adopted value of 29.531 derived from $\Delta_{fus}H°$ and $\Delta_f°$(Zn, g 298.15 K) = 31.1 ± 0.2 $kcal·mol^{-1}$. This difference of 0.059 $kcal·mol^{-1}$ is within the uncertainty of the vapor pressure studies.

The boiling point is calculated as that temperature for which $\Delta G° = 0$ for Zn(l) = Zn(g). T_{vap} is the temperature for which the fugacity is one bar.

References

References are listed on the Zn(cr, l) 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
	$J·K^{-1}mol^{-1}$			$kJ·mol^{-1}$			
0							
100							
200							
250							
298.15	25.387	50.792	50.792	0.	6.519	3.813	−0.668
300	25.406	50.949	50.793	0.047	6.519	3.796	−0.661
350	25.889	54.903	51.104	1.330	6.519	3.343	−0.499
400	26.346	58.390	51.801	2.636	6.519	2.889	−0.377
440.000	26.740	60.919	52.516	3.697	GLASS <--> LIQUID TRANSITION		
440.000	31.380	60.919	52.516	3.697			
450	31.380	61.624	52.711	4.011	6.565	2.435	−0.283
500	31.380	64.930	53.770	5.580	6.778	1.964	−0.205
600	31.380	70.652	56.122	8.718	7.119	0.967	−0.084
692.730	31.380	75.161	58.376	11.628	--- CRYSTAL <--> LIQUID ---		
700	31.380	75.489	58.552	11.856	0.	0.	0.
800	31.380	79.679	60.937	14.994	0.	0.	0.
900	31.380	83.375	63.228	18.132	0.	0.	0.
1000	31.380	86.681	65.411	21.270	0.	0.	0.
1100	31.380	89.672	67.483	24.408	0.	0.	0.
1180.173	31.380	91.880	69.066	26.924	----- FUGACITY = 1 bar -----		
1200	31.380	92.402	69.448	27.546	−115.101	1.935	−0.084
1300	31.380	94.914	71.311	30.684	−114.041	11.646	−0.468
1400	31.380	97.240	73.081	33.822	−112.982	21.274	−0.794
1500	31.380	99.405	74.765	36.960	−111.923	30.827	−1.073
1600	31.380	101.430	76.369	40.098	−110.863	40.309	−1.316
1700	31.380	103.332	77.899	43.236	−109.804	49.725	−1.528
1800	31.380	105.126	79.363	46.374	−108.744	59.078	−1.714
1900	31.380	106.823	80.764	49.512	−107.685	68.373	−1.880
2000	31.380	108.432	82.107	52.650	−106.626	77.612	−2.027

PREVIOUS: CURRENT: December 1978

J. Phys. Chem. Ref. Data, Monograph 9

0	to	692.73	K	crystal
above		692.73	K	liquid

Refer to the individual tables for details.

References for Zn(l) table

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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°	$-[G^\circ-H^\circ(T_r)]/T$	$H^\circ-H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K_f
0	0.	0.	INFINITE	−5.669	0.	0.	0.
100	19.455	16.523	63.224	−4.670	0.	0.	0.
200	24.050	31.820	44.005	−2.437	0.	0.	0.
250	25.039	37.290	42.132	−1.211	0.	0.	0.
298.15	25.387	41.717	41.717	0.	0.	0.	0.
300	25.406	41.874	41.717	0.047	0.	0.	0.
350	25.889	45.828	42.028	1.330	0.	0.	0.
400	26.346	49.314	42.725	2.636	0.	0.	0.
450	26.843	52.446	43.634	3.965	0.	0.	0.
500	27.386	55.301	44.660	5.321	0.	0.	0.
600	28.588	60.399	46.868	8.118	0.	0.	0.
692.730	29.802	64.591	48.965	10.825	CRYSTAL <--> LIQUID TRANSITION		
692.730	31.380	75.161	48.965	18.147			
700	31.380	75.489	49.239	18.375	0.	0.	0.
800	31.380	79.679	52.788	21.513	0.	0.	0.
900	31.380	83.375	55.985	24.651	0.	0.	0.
1000	31.380	86.681	58.892	27.789	0.	0.	0.
1100	31.380	89.672	61.557	30.927	0.	0.	0.
1180.173	31.380	91.880	63.542	33.443	----- FUGACITY = 1 bar -----		
1200	31.380	92.402	64.015	34.065	−115.101	1.936	−0.084
1300	31.380	94.914	66.297	37.203	−114.041	11.646	−0.468
1400	31.380	97.240	68.425	40.341	−112.982	21.274	−0.794
1500	31.380	99.405	70.419	43.479	−111.923	30.827	−1.073
1600	31.380	101.430	72.294	46.617	−110.863	40.309	−1.316
1700	31.380	103.332	74.065	49.755	−109.804	49.725	−1.528
1800	31.380	105.126	75.741	52.893	−108.744	59.078	−1.714
1900	31.380	106.823	77.333	56.031	−107.685	68.373	−1.880
2000	31.380	108.432	78.848	59.169	−106.626	77.612	−2.027

PREVIOUS: CURRENT. December 1978

IP(Zn, g) = 75768.10 ± 0.5 cm^{-1}
$S(298.15\ K) = 160.989 \pm 0.025\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 129.89 \pm 0.2\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 130.42 \pm 0.2\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
^1S_o	0	1
^3P_o	32311.308	1
$^3P_1$	32501.390	3
$^3P_2$	32890.317	5

Enthalpy of Formation

The adopted value for the enthalpy of formation is that recommended by CODATA.[1] This value is based on the reanalysis of the vapor pressure data cited by Hultgren *et al.*,[2] and Gurvich *et al.*[3] The studies by Mar and Searcy (512–666 K)[4] and McCreary and Thorn (610–690 K)[5] are also considered. There are twelve sublimation and eleven vaporization studies which lead to enthalpy of formation values showing excellent agreement, which the exception of two studies.

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Moore,[6] is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels (for $n<10$) and cutting off the summation in the partition function[7] has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state and the levels listed above; the next excited state is at approximately 46745 cm^{-1} above the ground state.

Although we list only a few electronic levels, all levels reported by Moore[6] are considered in the calculation. The reported uncertainty in $S°(298.15\ K)$ is due to uncertainties in he relative atomic mass and the fundamental constants. Extension of these calculations above 6000 K may require consideration of the excited states ($n>10$) and use of different fill and cutoff procedures.[7]

The thermal functions at 298.15 K differ from the CODATA recommendations[1] for two reasons. First, the entropy differs by 0.1094 $J \cdot K^{-1} \cdot mol^{-1}$ because this table uses a reference pressure of 1 bar, wheras CODATA recommendations are based on 1 atm. Second, small changes, ~0.004 $J \cdot K^{-1} \cdot mol^{-1}$, arise presumably due to the use of slightly different values for the fundamental constants.

References

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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
	$J \cdot K^{-1} \cdot mol^{-1}$			$kJ \cdot mol^{-1}$			
0	0.	0.	INFINITE	−6.197	129.892	129.892	INFINITE
100	20.786	138.281	179.469	−4.119	130.971	118.795	−62.052
200	20.786	152.689	162.890	−2.040	130.817	106.643	−27.852
250	20.786	157.327	161.331	−1.001	130.630	100.620	−21.023
298.15	20.786	160.989	160.989	0.	130.420	94.859	−16.619
300	20.786	161.117	160.989	0.038	130.411	94.638	−16.478
350	20.786	164.321	161.242	1.078	130.168	88.695	−13.237
400	20.786	167.097	161.804	2.117	129.902	82.788	−10.811
450	20.786	169.545	162.531	3.156	129.611	76.916	−8.928
500	20.786	171.735	163.344	4.196	129.295	71.078	−7.425
600	20.786	175.525	165.068	6.274	128.576	59.500	−5.180
700	20.786	178.729	166.797	8.353	120.398	48.130	−3.591
800	20.786	181.505	168.465	10.431	119.339	37.878	−2.473
900	20.786	183.953	170.053	12.510	118.279	27.759	−1.611
1000	20.786	186.143	171.554	14.589	117.220	17.758	−0.928
1100	20.786	188.124	172.972	16.667	116.160	7.863	−0.373
1180.173	20.786	189.586	174.052	18.334	----- FUGACITY = 1 bar -----		
1200	20.786	189.933	174.311	18.746	0.	0.	0.
1300	20.786	191.597	175.578	20.824	0.	0.	0.
1400	20.786	193.137	176.778	22.903	0.	0.	0.
1500	20.786	194.571	177.917	24.982	0.	0.	0.
1600	20.786	195.913	179.000	27.060	0.	0.	0.
1700	20.786	197.173	180.032	29.139	0.	0.	0.
1800	20.786	198.361	181.018	31.217	0.	0.	0.
1900	20.786	199.485	181.960	33.296	0.	0.	0.
2000	20.786	200.551	182.863	35.375	0.	0.	0.
2100	20.786	201.565	183.730	37.453	0.	0.	0.
2200	20.786	202.532	184.563	39.532	0.	0.	0.
2300	20.786	203.456	185.364	41.610	0.	0.	0.
2400	20.786	204.341	186.137	43.689	0.	0.	0.
2500	20.786	205.189	186.882	45.768	0.	0.	0.
2600	20.786	206.004	187.602	47.846	0.	0.	0.
2700	20.787	206.789	188.298	49.925	0.	0.	0.
2800	20.787	207.545	188.972	52.004	0.	0.	0.
2900	20.788	208.274	189.625	54.082	0.	0.	0.
3000	20.789	208.979	190.259	56.161	0.	0.	0.
3100	20.791	209.661	190.874	58.240	0.	0.	0.
3200	20.793	210.321	191.471	60.319	0.	0.	0.
3300	20.796	210.961	192.052	62.399	0.	0.	0.
3400	20.800	211.582	192.617	64.479	0.	0.	0.
3500	20.806	212.185	193.168	66.559	0.	0.	0.
3600	20.814	212.771	193.704	68.640	0.	0.	0.
3700	20.824	213.341	194.227	70.722	0.	0.	0.
3800	20.836	213.897	194.738	72.805	0.	0.	0.
3900	20.852	214.438	195.236	74.889	0.	0.	0.
4000	20.871	214.966	195.722	76.975	0.	0.	0.
4100	20.894	215.482	196.198	79.064	0.	0.	0.
4200	20.922	215.986	196.663	81.154	0.	0.	0.
4300	20.955	216.478	197.118	83.248	0.	0.	0.
4400	20.994	216.961	197.564	85.345	0.	0.	0.
4500	21.039	217.433	198.000	87.447	0.	0.	0.
4600	21.091	217.896	198.428	89.553	0.	0.	0.
4700	21.150	218.350	198.847	91.665	0.	0.	0.
4800	21.218	218.796	199.258	93.784	0.	0.	0.
4900	21.295	219.234	199.661	95.909	0.	0.	0.
5000	21.381	219.665	200.057	98.043	0.	0.	0.
5100	21.478	220.090	200.445	100.186	0.	0.	0.
5200	21.585	220.508	200.827	102.339	0.	0.	0.
5300	21.703	220.920	201.202	104.503	0.	0.	0.
5400	21.833	221.327	201.571	106.680	0.	0.	0.
5500	21.976	221.729	201.934	108.870	0.	0.	0.
5600	22.131	222.126	202.291	111.076	0.	0.	0.
5700	22.300	222.519	202.643	113.297	0.	0.	0.
5800	22.482	222.909	202.989	115.536	0.	0.	0.
5900	22.680	223.295	203.330	117.794	0.	0.	0.
6000	22.892	223.678	203.666	120.072	0.	0.	0.

PREVIOUS: December 1978 (1 atm) CURRENT. September 1984 (1 bar)

$IP(Zn^+, g) = 144892.6 \pm 2\ cm^{-1}$
$S°(298.15\ K) = 166.751 \pm 0.02\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 1030.6 \pm 0.84\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = [1037.336]\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2S_{1/2}$	0.0	2
$^2P_{1/2}$	48480.6	2
$^2P_{1/2}$	49354.4	4

Enthalpy of Formation

$\Delta_f H°(Zn^+, g, 0\ K)$ is calculated from $\Delta_f H°(Zn, g, 0\ K)$[1] using the spectroscopic value of $IP(Zn) = 75768.10 \pm 0.5\ cm^{-1}$ ($906.388 \pm 0.006\ kJ·mol^{-1}$) from Moore.[2] The ionization limit is converted from cm^{-1} to $kJ·mol^{-1}$ using the factor, $1\ cm^{-1} = 0.01196266\ kJ·mol^{-1}$, 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.

$\Delta_f H°(Zn^+, g, 298.15\ K)$ is calculated from $\Delta_f H°(Zn, g, 0\ K)$ by using IP(Zn) with JANAF[1] enthalpies, $H°(0\ K)$–$H°(298.15\ K)$, for Zn(g), $Zn^+(g)$, and e^-(ref). $\Delta_f H°(Zn \rightarrow Zn^+ + e^-, 298.15\ K)$ 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 Moore,[2,6] is incomplete because many theoretically predicted levels have not been observed. Our calculations indicate that any reasonable method of filling in these missing levels and cutting off the summation in the partition function[7] has no effect on the thermodynamic functions to 6000 K. This is a result of the high energy of all levels other than the ground state and the first two excited states; the next excited state is 62721.9 cm^{-1} above the ground state. Since inclusion of these excited states has no effect on the thermodynamic functions (to 6000 K), we list only the ground state and the first two excited states. 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 excited states and use of different fill and cutoff procedures.[7]

References

[1]JANAF Thermochemical Tables: Zn(g), 9–30–84; e^-(ref), 3–31–82.
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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	1030.611		
100	20.786	144.043	185.231	−4.119			
200	20.786	158.451	168.652	−2.040			
250	20.786	163.090	167.093	−1.001			
298.15	20.786	166.751	166.751	0.	1037.336	993.803	−174.110
300	20.786	166.879	166.751	0.038	1037.366	993.532	−172.989
350	20.786	170.083	167.004	1.078	1038.162	986.164	−147.177
400	20.786	172.859	167.566	2.117	1038.935	978.682	−127.803
450	20.786	175.307	168.293	3.156	1039.684	971.105	−112.723
500	20.786	177.497	169.106	4.196	1040.407	963.446	−100.651
600	20.786	181.287	170.830	6.274	1041.767	947.925	−82.524
700	20.786	184.491	172.559	8.353	1035.667	932.262	−69.566
800	20.786	187.267	174.227	10.431	1036.686	917.420	−59.901
900	20.786	189.715	175.815	12.510	1037.705	902.451	−52.377
1000	20.786	191.905	177.316	14.589	1038.725	887.368	−46.351
1100	20.786	193.886	178.734	16.667	1039.744	872.183	−41.417
1200	20.786	195.695	180.073	18.746	925.662	858.840	−37.384
1300	20.786	197.359	181.340	20.824	927.741	853.188	−34.282
1400	20.786	198.899	182.540	22.903	929.819	847.375	−31.616
1500	20.786	200.333	183.679	24.982	931.898	841.413	−29.301
1600	20.786	201.675	184.762	27.060	933.977	835.313	−27.270
1700	20.786	202.935	185.794	29.139	936.055	829.083	−25.475
1800	20.786	204.123	186.780	31.217	938.134	822.731	−23.875
1900	20.786	205.247	187.722	33.296	940.212	816.263	−22.441
2000	20.786	206.313	188.626	35.375	942.291	809.685	−21.147
2100	20.786	207.327	189.492	37.453	944.370	803.004	−19.974
2200	20.786	208.294	190.325	39.532	946.448	796.224	−18.905
2300	20.786	209.218	191.126	41.610	948.527	789.349	−17.927
2400	20.786	210.103	191.899	43.689	950.605	782.383	−17.028
2500	20.786	210.951	192.644	45.768	952.684	775.331	−16.200
2600	20.786	211.766	193.364	47.846	954.763	768.196	−15.433
2700	20.786	212.551	194.060	49.925	956.841	760.981	−14.722
2800	20.786	213.307	194.734	52.004	958.920	753.689	−14.060
2900	20.786	214.036	195.387	54.082	960.998	746.323	−13.443
3000	20.786	214.741	196.021	56.161	963.077	738.885	−12.865
3100	20.786	215.422	196.636	58.239	965.155	731.377	−12.324
3200	20.786	216.082	197.233	60.318	967.233	723.803	−11.815
3300	20.786	216.722	197.814	62.397	969.311	716.164	−11.336
3400	20.786	217.343	198.379	64.475	971.388	708.461	−10.884
3500	20.786	217.945	198.930	66.554	973.465	700.698	−10.457
3600	20.786	218.531	199.466	68.632	975.541	692.875	−10.053
3700	20.786	219.100	199.989	70.711	977.616	684.995	−9.670
3800	20.786	219.654	200.499	72.790	979.691	677.058	−9.307
3900	20.786	220.194	200.997	74.868	981.763	669.067	−8.961
4000	20.786	220.721	201.484	76.947	983.835	661.023	−8.632
4100	20.786	221.234	201.959	79.025	985.904	652.927	−8.318
4200	20.786	221.735	202.424	81.104	987.970	644.781	−8.019
4300	20.787	222.224	202.879	83.183	990.033	636.585	−7.733
4400	20.787	222.702	203.324	85.261	992.093	628.342	−7.459
4500	20.787	223.169	203.760	87.340	994.149	620.051	−7.197
4600	20.787	223.626	204.187	89.419	996.200	611.716	−6.946
4700	20.788	224.073	204.605	91.497	998.245	603.335	−6.705
4800	20.788	224.511	205.015	93.576	1000.284	594.911	−6.474
4900	20.789	224.939	205.418	95.655	1002.316	586.445	−6.252
5000	20.790	225.359	205.812	97.734	1004.340	577.937	−6.038
5100	20.791	225.771	206.200	99.813	1006.355	569.389	−5.832
5200	20.792	226.175	206.580	101.892	1008.360	560.802	−5.633
5300	20.794	226.571	206.953	103.972	1010.353	552.176	−5.442
5400	20.796	226.959	207.320	106.051	1012.334	543.512	−5.257
5500	20.798	227.341	207.681	108.131	1014.302	534.812	−5.079
5600	20.800	227.716	208.035	110.211	1016.256	526.076	−4.907
5700	20.803	228.084	208.384	112.291	1018.193	517.306	−4.741
5800	20.807	228.446	208.727	114.371	1020.113	508.502	−4.580
5900	20.811	228.801	209.064	116.452	1022.015	499.665	−4.424
6000	20.815	229.151	209.396	118.533	1023.896	490.795	−4.273

PREVIOUS. December 1978 (1 atm) CURRENT: September 1984 (1 bar)

EA(Zn, g) = 0.9 ± 0.20 eV
$S°$(298.15 K) = 160.99 ± 0.03 J·K^{-1}·mol^{-1}

$\Delta_f H°$(0 K) = 115.5 ± 20 kJ·mol^{-1}
$\Delta_f H°$(298.15 K) = [109.870] kJ·mol^{-1}

Electonic Level and Quantum Weight		
State	ϵ_i, cm^{-1}	g_i
$^2S_{1/2}$	0	2

Enthalpy of Formation

$\Delta_f H°(Zn^-, g, 0 K)$ is calculated from $\Delta_f H°(Zn, g, 0 K)$[1] using the adopted electron affinity of EA(Zn) = 0.09 ± 0.20 eV − 0.67 ± 19.3 kJ·mol^{-1}). This value is calculated by Zollwig[2] using a horizontal analysis technique for the ground state $3d^{10}4s^25s(^2S_{1/2})$. There is a possibility that the ground state may be $3d^{10}4s^24p$ (^2P_o) in which case Zollwig[2] calculated an electron affinity EA = −0.67 eV. Hotop and Lineberger,[3] in a recent review, recommends that $Zn^-(g)$ has a metastable state, $4s4p^24p$, with EA>0.[2,4] Additional information on Zn^- may be obtained in the critical discussions of Hotop and Lineberger,[3,4] Rosenstock *et al.*,[6] and Massey;[7] and in the articles by Gohel *et al.*[8] and Kaiser *et al.*[9]

$\Delta_f H°(Zn^-, g, 298.15 K)$ is obtained from $\Delta_f H°(Zn, g, 0 K)$ by using EA(Zn) with JANAF[1] enthalpies, $H°(0 K)$–$H°(298.15 K)$, for $Zn^-(g)$, Zn(g), and e^-(ref). $\Delta_r H°(Zn^- \rightarrow Zn + e^-, 298.15 K)$ differs from a room-temperature threshold energy due to inclusion of these enthalpies and to threshold effects discussed by Rosenstock *et al.*[6] $\Delta_f H°(298.15 K)$ 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 $Zn^-(g)$ is that given by Zollwig.[2] Lacking any experimental evidence as to the stability of any excited states, we assume that no stable states exist.

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[1]JANAF Thermocemical Tables: Zn(g), 9–30–84; e^-(g), 3–31–82.
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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	−6.197	115.539		
100	20.786	138.282	179.469	−4.119			
200	20.786	152.689	162.890	−2.040			
250	20.786	157.328	161.331	−1.001			
298.15	20.786	160.989	160.989	0.	109.870	80.564	−14.114
300	20.786	161.117	160.989	0.038	109.823	80.382	−13.996
350	20.786	164.321	161.242	1.078	108.540	75.576	−11.279
400	20.786	167.097	161.804	2.117	107.234	70.956	−9.266
450	20.786	169.545	162.531	3.156	105.905	66.501	−7.719
500	20.786	171.735	163.344	4.196	104.549	62.195	−6.497
600	20.786	175.525	165.068	6.274	101.752	53.985	−4.700
700	20.786	178.729	166.797	8.353	91.495	46.330	−3.457
800	20.786	181.505	168.466	10.431	88.357	40.092	−2.618
900	20.786	183.953	170.053	12.510	85.219	34.247	−1.988
1000	20.786	186.143	171.554	14.589	82.081	28.752	−1.502
1100	20.786	188.124	172.972	16.667	78.943	23.571	−1.119
1200	20.786	189.933	174.311	18.746	−39.296	20.611	−0.897
1300	20.786	191.597	175.578	20.824	−41.374	25.688	−1.032
1400	20.786	193.137	176.778	22.903	−43.453	30.924	−1.154
1500	20.786	194.571	177.917	24.982	−45.532	36.310	−1.264
1600	20.786	195.913	179.000	27.060	−47.610	41.834	−1.366
1700	20.786	197.173	180.032	29.139	−49.689	47.487	−1.459
1800	20.786	198.361	181.018	31.217	−51.767	53.264	−1.546
1900	20.786	199.485	181.960	33.296	−53.846	59.155	−1.626
2000	20.786	200.551	182.864	35.375	−55.925	65.157	−1.702
2100	20.786	201.565	183.730	37.453	−58.003	71.262	−1.773
2200	20.786	202.532	184.563	39.532	−60.082	77.466	−1.839
2300	20.786	203.456	185.364	41.610	−62.160	83.765	−1.902
2400	20.786	204.341	186.137	43.689	−64.239	90.154	−1.962
2500	20.786	205.189	186.882	45.768	−66.318	96.630	−2.019
2600	20.786	206.004	187.602	47.846	−68.396	103.189	−2.073
2700	20.786	206.789	188.298	49.925	−70.475	109.827	−2.125
2800	20.786	207.545	188.972	52.004	−72.554	116.543	−2.174
2900	20.786	208.274	189.625	54.082	−74.632	123.334	−2.221
3000	20.786	208.979	190.259	56.161	−76.711	130.195	−2.267
3100	20.786	209.660	190.874	58.239	−78.790	137.127	−2.311
3200	20.786	210.320	191.471	60.318	−80.869	144.125	−2.353
3300	20.786	210.960	192.052	62.397	−82.949	151.188	−2.393
3400	20.786	211.581	192.617	64.475	−85.029	158.314	−2.432
3500	20.786	212.183	193.168	66.554	−87.109	165.502	−2.470
3600	20.786	212.769	193.704	68.632	−89.190	172.749	−2.507
3700	20.786	213.338	194.227	70.711	−91.272	180.053	−2.542
3800	20.786	213.892	194.737	72.790	−93.355	187.414	−2.576
3900	20.786	214.432	195.235	74.868	−95.439	194.830	−2.609
4000	20.786	214.959	195.722	76.947	−97.525	202.299	−2.642
4100	20.786	215.472	196.197	79.025	−99.614	209.821	−2.673
4200	20.786	215.973	196.662	81.104	−101.704	217.393	−2.704
4300	20.786	216.462	197.117	83.183	−103.798	225.016	−2.733
4400	20.786	216.940	197.562	85.261	−105.895	232.687	−2.762
4500	20.786	217.407	197.998	87.340	−107.997	240.406	−2.791
4600	20.786	217.864	198.425	89.418	−110.103	248.171	−2.818
4700	20.786	218.311	198.843	91.497	−112.215	255.982	−2.845
4800	20.786	218.748	199.253	93.576	−114.334	263.839	−2.871
4900	20.786	219.177	199.656	95.654	−116.459	271.739	−2.897
5000	20.786	219.597	200.050	97.733	−118.593	279.683	−2.922
5100	20.786	220.009	200.438	99.811	−120.736	287.670	−2.946
5200	20.786	220.412	200.818	101.890	−122.889	295.699	−2.970
5300	20.786	220.808	201.191	103.969	−125.053	303.770	−2.994
5400	20.786	221.197	201.558	106.047	−127.230	311.881	−3.017
5500	20.786	221.578	201.919	108.126	−129.420	320.033	−3.039
5600	20.786	221.953	202.273	110.204	−131.626	328.224	−3.062
5700	20.786	222.320	202.622	112.283	−133.847	336.456	−3.083
5800	20.786	222.682	202.964	114.362	−136.086	344.726	−3.105
5900	20.786	223.037	203.302	116.440	−138.344	353.035	−3.126
6000	20.786	223.387	203.634	118.519	−140.622	361.383	−3.146

PREVIOUS: December 1978 (1 atm) CURRENT: September 1984 (1 bar)