$S°(298.15\ K) = 76.03 \pm 0.2\ J\ K^{-1}\cdot mol^{-1}$
$T_{fus} = 234.29\ K$

$\Delta_f H°(0\ K) = 0\ kJ\ mol^{-1}$
$\Delta_f H°(298.15\ K) = 0\ kJ\cdot mol^{-1}$
$\Delta_{fus} H° = 2.2953 \pm 0.0004\ kJ\cdot mol^{-1}$

Enthalpy of Formation

Zero by definition.

Heat Capacity and Entropy

The heat capacities of Smith and Wolcott, (1.2-20 2 K),[1] Busey and Giaugue (15-330 K),[2] and Douglas *et al.* (300-770 K),[3] have been smoothly joined. There is fair agreement between the selected values and those of Pickard and Simon,[4] Carpenter and Oakley,[5] Carpenter and Stoodley,[6] Cohen *et al.*,[7] Dixon and Rodebush,[8] Simon,[9] Bronsted,[10] and Pollitzer.[11]

Fusion Data

The results of Busey and Giauque[2] are adopted.

Vaporization Data

Refer to the gas phase tables for details.

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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	−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			
250	28.351	71.069	76.490	−1.355	0.	0.	0.
298.15	27.978	76.028	76.028	0.	0.	0.	0.
300	27.963	76.201	76.028	0.052	0.	0.	0.
350	27.639	80.486	76.368	1.441	0.	0.	0.
400	27.414	84.161	77.118	2.817	0.	0.	0.
450	27.267	87.381	78.083	4.184	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	FUGACITY = 1 bar		
700	27.291	99.389	83.705	10.979	−58 754	6.571	−0 490
800	27.582	103.052	85.899	13.722	−58.089	15.858	−1.035
900	27.896	106.318	87.990	16.496	−57.394	25.060	−1 454
1000	28.210	109.274	89.973	19.301	−56.667	34.183	−1.786
1100	28.523	111.977	91.852	22.138	−55.909	43.232	−2.053
1200	28.837	114.472	93.634	25.006	−55.120	52.210	−2.273
1300	29.151	116.793	95.328	27.905	−54.299	61.121	−2.456
1400	29.465	118.965	96.939	30.836	−53.447	69.968	−2.611
1500	29.778	121.008	98.476	33.798	−52.563	78.752	−2.742
1600	30.092	122.940	99.945	36.792	−51.649	87.477	−2.856
1700	30.406	124.774	101.352	39.816	−50.702	96.144	−2.954
1800	30 719	126.521	102.703	42.873	−49.725	104.754	−3.040
1900	31.033	128.190	104.000	45.960	−48.716	113.308	−3.115
2000	31.347	129.790	105.250	49.079	−47.675	121.809	−3 181

PREVIOUS: CURRENT: December 1961

IP(Hg, g) = 84184.1 ± 0.5 cm^{-1}
$S°(298.15\ K) = 174.970 \pm 0.020\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = 64.53 \pm 0.04\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = 61.38 \pm 0.04\ kJ \cdot mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^1S_0$	0.000	1
$^3P_0$	37645.080	1
$^3P_1$	39412.300	3
$^3P_2$	44042.977	5

Enthalpy of Formation

The value adopted for the enthalpy of formation of Hg(g) is that recommended by CODATA.[1] This value was derived from the vapor pressure studies summarized by Hultgren *et al.*[2] Of the 24 studies examined, most weight was given to the following studies: Spedding and Dye (533–630 K),[3] Menzies (395 625 K),[4] Beattie *et al.* (623–635 K),[5] Burlingame (343–474 K),[6] Rodebush and Dixon (444–476 K),[7] and Mayer (262–298 K).[8]

Heat Capacity and Entropy

The information on electronic energy levels and quantum weights, given by Moore,[9,10] 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[11] 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 three levels below 45000 cm^{-1}; the next excited state is approximately 54000 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 three P levels. 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.[11]

The thermal functions at 298.15 K agree with the CODATA recommendations[1] except that the entropy differs by 0.1094 $J \cdot K^{-1} \cdot mol^{-1}$, since this table uses a standard state pressure of 1 bar (CODATA recommendations are based on 1 atm).

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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
	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
0	0.	0.	INFINITE	−6.197	64.526	64.526	INFINITE
100	20.786	152.263	193.450	−4.119	64.899	53.394	−27.890
200	20.786	166.670	176.871	−2.040	64.392	42.062	−10.986
250	20.786	171.309	175.312	−1.001	61.735	36.675	−7.663
298.15	20.786	174.970	174.970	0.	61.380	31.880	−5.585
300	20.786	175.098	174.970	0.038	61.367	31.697	−5.519
350	20.786	178.303	175.223	1.078	61.016	26.781	−3.997
400	20.786	181.078	175.786	2.117	60.680	21.913	−2.862
450	20.786	183.526	176.512	3.156	60.352	17.087	−1.983
500	20.786	185.717	177.325	4.196	60.031	12.297	−1.285
600	20.786	189.506	179.049	6.274	59.395	2.810	−0.245
629.839	20.786	190.515	179.569	6.894	----- FUGACITY = 1 bar -----		
700	20.786	192.710	180.778	8.353	0	0.	0.
800	20.786	195.486	182.447	10.431	0	0.	0.
900	20.786	197.934	184.034	12.510	0.	0.	0.
1000	20.786	200.124	185.536	14.589	0.	0.	0.
1100	20.786	202.105	186.953	16.667	0.	0.	0.
1200	20.786	203.914	188.292	18.746	0.	0.	0.
1300	20.786	205.578	189.559	20.824	0.	0.	0.
1400	20.786	207.118	190.759	22.903	0.	0.	0.
1500	20.786	208.552	191.898	24.982	0.	0.	0.
1600	20.786	209.894	192.981	27.060	0.	0.	0.
1700	20.786	211.154	194.013	29.139	0.	0.	0.
1800	20.786	212.342	194.999	31.217	0.	0	0
1900	20.786	213.466	195.942	33.296	0.	0.	0.
2000	20.786	214.532	196.845	35.375	0.	0.	0
2100	20.786	215.546	197.711	37.453	0.	0.	0
2200	20.786	216.513	198.544	39.532	0.	0.	0.
2300	20.786	217.437	199.346	41.610	0.	0.	0.
2400	20.786	218.322	200.118	43.689	0.	0.	0.
2500	20.786	219.170	200.863	45.768	0.	0.	0
2600	20.786	219.986	201.583	47.846	0.	0.	0.
2700	20.786	220.770	202.279	49.925	0.	0	0.
2800	20.786	221.526	202.953	52.004	0.	0.	0.
2900	20.786	222.255	203.606	54.082	0.	0	0.
3000	20.786	222.960	204.240	56.161	0.	0.	0.
3100	20.786	223.642	204.855	58.239	0.	0.	0.
3200	20.786	224.302	205.452	60.318	0.	0	0.
3300	20.787	224.941	206.033	62.397	0.	0.	0.
3400	20.787	225.562	206.598	64.475	0.	0.	0.
3500	20.787	226.164	207.149	66.554	0.	0.	0.
3600	20.788	226.750	207.685	68.633	0.	0.	0.
3700	20.789	227.319	208.208	70.712	0.	0.	0.
3800	20.790	227.874	208.719	72.790	0.	0.	0.
3900	20.791	228.414	209.217	74.869	0.	0.	0.
4000	20.793	228.940	209.703	76.949	0.	0.	0.
4100	20.795	229.454	210.179	79.028	0.	0.	0.
4200	20.798	229.955	210.644	81.108	0.	0.	0.
4300	20.802	230.444	211.098	83.188	0.	0.	0.
4400	20.807	230.923	211.544	85.268	0.	0.	0.
4500	20.813	231.390	211.979	87.349	0.	0.	0.
4600	20.820	231.848	212.406	89.431	0.	0.	0.
4700	20.829	232.296	212.825	91.513	0.	0.	0.
4800	20.839	232.734	213.235	93.597	0.	0.	0.
4900	20.851	233.164	213.637	95.681	0.	0.	0.
5000	20.866	233.586	214.032	97.767	0.	0.	0.
5100	20.882	233.999	214.420	99.855	0.	0.	0.
5200	20.902	234.405	214.800	101.944	0.	0.	0.
5300	20.924	234.803	215.174	104.035	0.	0.	0.
5400	20.949	235.194	215.541	106.129	0.	0.	0.
5500	20.978	235.579	215.902	108.225	0.	0	0.
5600	21.010	235.957	216.256	110.324	0.	0.	0.
5700	21.046	236.329	216.605	112.427	0.	0	0.
5800	21.087	236 696	216.949	114.534	0.	0.	0.
5900	21.132	237.057	217.286	116.644	0.	0.	0.
6000	21 182	237.412	217.619	118.760	0.	0.	0.

PREVIOUS December 1961 (1 atm) CURRENT September 1984 (1 bar)

Mercury, Ion (Hg^+)

IDEAL GAS

$M_r = 200.58945$ **Mercury, Ion (Hg^+)**

$Hg^+_1(g)$

$IP(Hg^+, g) = 151280 \pm 10\ cm^{-1}$
$S°(298.15\ K) = 224.617 \pm 0.025\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 1071.57 \pm 4.0\ kJ·mol^{-1}$
$\Delta_f H°(298.15\ K) = [1074.623]\ kJ·mol^{-1}$

Electronic Levels and Quantum Weights		
State	ϵ_i, cm^{-1}	g_i
$^2S_{1/2}$	0	2
$^2D_{5/2}$	35514	6
$^2D_{3/2}$	50552	4
$^2P_{1/2}$	51485	2
$^2P_{3/2}$	60608	4

Enthalpy of Formation

$\Delta_f H°(Hg^+, g, 0\ K)$ is calculated from $\Delta_f H°(Hg, g, 0\ K)$[1] using the spectroscopic value of IP(Hg) = 84184.1 ± 0.5 cm^{-1}(1007.066 ± 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.

$\Delta_f H°(Hg^+, g, 298.15\ K)$ is calculated from $\Delta_f H°(Hg, g, 0\ K)$ by using IP(Hg) with JANAF[1] enthalpies, $H°(0\ K)–H°(298.15\ K)$, for Hg(g), $Hg^+(g)$, and e^-(ref). $\Delta_f H°(Hg \rightarrow Hg^+ + e^-, 298.15\ K)$ 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 of the summation in the partition functions[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 four excited states; the next excited state is approximately 79704 cm^{-1} above the ground state. Since inclusion of these excited states has no effect on the thermodynamic functions (to 6000), we list only the ground state and the first four 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]

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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	−6.197	1071.571		
100	20.786	158.026	199.213	−4.119			
150	20.786	166.454	186.983	−3.079			
200	20.786	172.434	182.634	−2.040			
250	20.786	177.072	181.075	−1.001			
298.15	20.786	180.733	180.733	.000	1074.623	1037.151	−181.704
300	20.786	180.862	180.733	.038	1074.648	1036.918	−180.543
350	20.786	184.066	180.986	1.078	1075.337	1030.575	−153.805
400	20.786	186.841	181.549	2.117	1076.040	1024.133	−133.738
450	20.786	189.290	182.275	3.156	1076.752	1017.602	−118.120
500	20.786	191.480	183.088	4.196	1077.470	1010.991	−105.618
600	20.786	195.269	184.812	6.274	1078.913	997.560	−86.845
700	20.786	198.474	186.541	8.353	1021.596	990.459	−73.909
800	20.786	201.249	188.210	10.431	1023.675	985.868	−64.371
900	20.786	203.697	189.797	12.510	1025.753	981.018	−56.937
1000	20.786	205.887	191.299	14.589	1027.832	975.936	−50.978
1100	20.786	207.869	192.716	16.667	1029.911	970.646	−46.092
1200	20.786	209.677	194.056	18.746	1031.989	965.166	−42.013
1300	20.786	211.341	195.322	20.824	1034.068	959.513	−38.554
1400	20.786	212.881	196.522	22.903	1036.146	953.700	−35.583
1500	20.786	214.315	197.661	24.982	1038.225	947.739	−33.003
1600	20.786	215.657	198.744	27.060	1040.304	941.639	−30.741
1700	20.786	216.917	199.777	29.139	1042.382	935.408	−28.742
1800	20.786	218.105	200.762	31.217	1044.461	929.056	−26.960
1900	20.786	219.229	201.705	33.296	1046.539	922.588	−25.364
2000	20.786	220.295	202.608	35.375	1048.618	916.010	−23.924
2100	20.786	221.309	203.474	37.453	1050.697	909.329	−22.618
2200	20.786	222.276	204.307	39.532	1052.775	902.548	−21.429
2300	20.786	223.200	205.109	41.611	1054.854	895.673	−20.341
2400	20.786	224.085	205.881	43.689	1056.932	888.708	−19.342
2500	20.786	224.933	206.626	45.768	1059.011	881.656	−18.421
2600	20.786	225.749	207.346	47.846	1061.090	874.520	−17.569
2700	20.786	226.533	208.042	49.925	1063.168	867.305	−16.779
2800	20.786	227.289	208.716	52.004	1065.247	860.013	−16.044
2900	20.786	228.019	209.369	54.082	1067.325	852.646	−15.358
3000	20.786	228.723	210.003	56.161	1069.404	845.208	−14.716
3100	20.787	229.405	210.618	58.239	1071.483	837.701	−14.115
3200	20.787	230.065	211.215	60.318	1073.561	830.126	−13.550
3300	20.787	230.704	211.796	62.397	1075.640	822.487	−13.019
3400	20.788	231.325	212.362	64.476	1077.719	814.784	−12.518
3500	20.788	231.928	212.912	66.554	1079.797	807.021	−12.044
3600	20.789	232.513	213.448	68.633	1081.876	799.198	−11.596
3700	20.791	233.083	213.971	70.712	1083.955	791.317	−11.171
3800	20.793	233.637	214.482	72.791	1086.034	783.380	−10.768
3900	20.795	234.177	214.980	74.871	1088.113	775.388	−10.385
4000	20.798	234.704	215.466	76.950	1090.192	767.343	−10.020
4100	20.801	235.218	215.942	79.030	1092.271	759.246	−9.673
4200	20.805	235.719	216.407	81.111	1094.350	751.099	−9.341
4300	20.811	236.208	216.862	83.191	1096.429	742.901	−9.024
4400	20.817	236.687	217.307	85.273	1098.509	734.656	−8.721
4500	20.824	237.155	217.743	87.355	1100.589	726.363	−8.431
4600	20.833	237.613	218.170	89.438	1102.668	718.024	−8.153
4700	20.843	238.061	218.588	91.521	1104.748	709.640	−7.887
4800	20.855	238.500	218.998	93.606	1106.828	701.211	−7.631
4900	20.868	238.930	219.401	95.693	1108.909	692.739	−7.385
5000	20.883	239.352	219.796	97.780	1110.989	684.225	−7.148
5100	20.901	239.765	220.183	99.869	1113.069	675.669	−6.920
5200	20.920	240.171	220.564	101.960	1115.150	667.072	−6.701
5300	20.942	240.570	220.937	104.053	1117.230	658.435	−6.489
5400	20.966	240.962	221.305	106.149	1119.311	649.759	−6.285
5500	20.993	241.347	221.665	108.247	1121.391	641.045	−6.088
5600	21.022	241.725	222.020	110.347	1123.471	632.292	−5.898
5700	21.054	242.098	222.369	112.451	1125.550	623.503	−5.714
5800	21.089	242.464	222.713	114.558	1127.630	614.677	−5.536
5900	21.127	242.825	223.050	116.669	1129 708	605.815	−5.363
6000	21.168	243.180	223.383	118.784	1131.786	596.918	−5.197

PREVIOUS — CURRENT: September 1984 (1 bar)

$S°(298.15\ K) = 280.752\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = 138.82\ kJ·mol^{-1}$

$\Delta_f H°(298.15\ K) = 133.47 \pm 4.6\ kJ·mol^{-1}$

Electronic Level and Quantum Weight		
State	ϵ_i, cm^{-1}	g_i
$^2\Sigma$	0	2

$\omega_e = 125.0\ cm^{-1}$ $\omega_e x_e = 1.00\ cm^{-1}$ $\sigma = 1$

$B_e = [0.0351]\ cm^{-1}$ $\alpha_e = [0.0003]\ cm^{-1}$ $r_e = [2.49]$ Å

Enthalpy of Formation

Wieland and Herczog[1] gave 8.3 ± 1.1 kcal·mol^{-1} for the enthalpy of dissociation into gaseous atoms.

Heat Capacity and Entropy

Vibrational constants were taken from Wieland.[2] Rotational constants are estimated using equation III–123 in Herzberg.[3] The bond length was estimated to be 0.965 of the mercuric bond length by analogy with the mercury chlorides.

References

[1]K. Wieland and A Herczog, Helv. Chim. Acta, 32, 889, (1949).
[2]K. Wieland, Zeits, F. Electrochemie 64, 761 (1960).
[3]G. Herzberg, "Spectra of Diatomic Molecules," D. van Nostrand, New York, (1950); refer to p 108.

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	−10.595	138.817	138.817	INFINITE
100	35.757	240.288	314.043	−7.375	138.805	121.548	−63.490
200	37.382	265.715	284.205	−3.698	137.432	104.789	−27.368
250	37.696	274.092	281.375	−1.821	134.298	96.877	−20.241
298.15	37.919	280.752	280.752	0.	133.470	89.745	−15.723
300	37.926	280.986	280.752	0.070	133.438	89.474	−15.579
350	38.116	286.847	281.215	1.971	132.543	82.216	−12.270
400	38.284	291.948	282.245	3.881	123.664	75.362	−9.841
450	38.438	296.466	283.578	5.799	122.199	69.412	−8.057
500	38.585	300.524	285.074	7.725	100.682	65.524	−6.845
600	38.864	307.583	288.254	11.598	99.964	58.561	−5.098
700	39.132	313.594	291.455	15.497	40.506	58.287	−4.349
800	39.394	318.837	294.557	19.424	40.464	60.830	−3.972
900	39.653	323.492	297.518	23.376	40.443	63.377	−3.678
1000	39.910	327.683	300.329	27.354	40.441	65.926	−3.444
1100	40.166	331.499	302.992	31.358	40.459	68.474	−3.252
1200	40.420	335.005	305.515	35.387	40.493	71.019	−3.091
1300	40.674	338.250	307.910	39.442	40.541	73.561	−2.956
1400	40.928	341.274	310.186	43.522	40.599	76.099	−2.839
1500	41.181	344.106	312.354	47.628	40.663	78.633	−2.738
1600	41.434	346.772	314.423	51.759	40.726	81.162	−2.650
1700	41.687	349.291	316.400	55.915	40.786	83.687	−2.571
1800	41.940	351.681	318.295	60.096	40.838	86.209	−2.502
1900	42.192	353.956	320.112	64.303	40.881	88.729	−2.439
2000	42.444	356.126	321.859	68.534	40.914	91.246	−2.383
2100	42.697	358.203	323.541	72.791	40.938	93 762	−2.332
2200	42.949	360.195	325.162	77.074	40.957	96.277	−2.286
2300	43.201	362.110	326.727	81.381	40.973	98.791	−2.244
2400	43.453	363.954	328.240	85.714	40.992	101.305	−2.205
2500	43.705	365 733	329.704	90.072	41.020	103.817	−2.169
2600	43.957	367.452	331.123	94.455	41.061	106.328	−2.136
2700	44.209	369.116	332.500	98.863	41.122	108.838	−2.106
2800	44.461	370.728	333.836	103.297	41.209	111.344	−2.077
2900	44.713	372.293	335.136	107.756	41.327	113.847	−2.051
3000	44.965	373.813	336.400	112.239	41.481	116.345	−2.026
3100	45.217	375.291	337.630	116.749	41.674	118.837	−2.002
3200	45.469	376.731	338.830	121.283	41.912	121.323	−1.980
3300	45.721	378.134	340.000	125.842	42.196	123.800	−1.960
3400	45.973	379.502	341.142	130.427	42.530	126.268	−1.940
3500	46.225	380.839	342.257	135.037	42.915	128.726	−1.921
3600	46.476	382.144	343.347	139.672	43.352	131.171	−1.903
3700	46.728	383.421	344.413	144.332	43.844	133.604	−1.886
3800	46.980	384.671	345.456	149.018	44.389	136.023	−1.870
3900	47.232	385.894	346.477	153.728	44.990	138.427	−1.854
4000	47.484	387.093	347.477	158.464	45.645	140.814	−1.839
4100	47.736	388.269	348.458	163.225	46.355	143.185	−1.824
4200	47.988	389.422	349.420	168.011	47 119	145.537	−1.810
4300	48.239	390.554	350.363	172.823	47.936	147.871	−1.796
4400	48.491	391.666	351.289	177.659	48.806	150.185	−1.783
4500	48.743	392.759	352.199	182.521	49.729	152.479	−1.770
4600	48.995	393.833	353.092	187.408	50.702	154.751	−1.757
4700	49.247	394.889	353.970	192.320	51.726	157.003	−1.745
4800	49.498	395.929	354.834	197.257	52.799	159.231	−1.733
4900	49.750	396.952	355.683	202.219	53.920	161.437	−1.721
5000	50.002	397.960	356.518	207.207	55.088	163.619	−1.709
5100	50.254	398.952	357.341	212.220	56.302	165.778	−1.698
5200	50.506	399.931	358.150	217.258	57.561	167.913	−1.687
5300	50.757	400.895	358.948	222.321	58.864	170.022	−1.676
5400	51.009	401.846	359.733	227.409	60.210	172.107	−1.665
5500	51.261	402.784	360.507	232.523	61.598	174.166	−1.654
5600	51.513	403.710	361.271	237.661	63.025	176.201	−1.644
5700	51.765	404.624	362.023	242.825	64.493	178.208	−1.633
5800	52.016	405.527	362.766	248.014	65.998	180.190	−1.623
5900	52.268	406.418	363.498	253.229	67.541	182.146	−1.613
6000	52.520	407.299	364.221	258.468	69.120	184.075	−1.603

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

$S°(298\ 15\ K)$ = [181.326 ± 6.3] $J·K^{-1}·mol^{-1}$
T_{trs} = 402 K
T_{fus} = 530 K

$\Delta_f H°(298.15\ K) = -105.437 \pm 1.7\ kJ·mol^{-1}$
$\Delta_{trs}H° = 2.515 \pm 0.17\ kJ·mol^{-1}$
$\Delta_{fus}H° = 18.966 \pm 0.21\ kJ·mol^{-1}$

Enthalpy of Formation

The value recommended by NBS[1] is adopted.

Heat Capacity and Entropy

The heat capacity is calculated from the enthalpy data of Guinchant[2] and Ewald.[3] The entropy is estimated by adjusting its value to provide the best fit of the melting, sublimation and vaporization phenomena.

Transition and Fusion Data

The enthalpy of transition, $\Delta_{trs}H° = 0.601 \pm 0.04$ kcal·mol^{-1}, and the temperature of transition are taken from NBS.[1] The enthalpy of melting, $\Delta_{fus}H° = 4.533 \pm 0.05$ kcal·mol^{-1} was taken from Guinchant,[2] the temperature of melting from NBS.[1]

References

[1]U S. Nat. Bur. Stand. Circ. 500, 1268 pp. (1952).
[2]M. Guinchant, Comp. Rend. 68, 145 (1907).
[3]R. Ewald, Ann. d. Physik (4) 44, 1213 (1914).

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							
100							
200							
250							
298.15	77.747	181.326	181.326	0	−105.437	−102.204	17.906
300	77.822	181.807	181.328	0.144	−105.445	−102 184	17.792
400	82.006	204.768	184.430	8.135	−121.858	−100.476	13.121
402.000	82.090	205.178	184.532	8.299	I <--> II		
402.000	84.119	211.433	184.532	10.814	TRANSITION		
500	84.119	229 784	191.669	19.058	−161.859	−91.667	9.576
530.000	84.119	234.686	193.966	21.581	----- II <--> LIQUID -----		
600	84.119	245.121	199.338	27.470	−159 916	−77.812	6.774
700	84.119	258.088	206.828	35.882	−216.745	−57 709	4.306
800	84.119	269.320	213.954	44.294	−214.191	−35.164	2.296
900	84 119	279.228	220.667	52.705	−211.648	−12.939	0.751
1000	84.119	288.091	226.974	61.117	−209.116	9.004	−0.470
1100	84.119	296.109	232.900	69.529	−206.598	30.694	−1.458
1200	84.119	303.428	238.477	77.941	−204.098	52.156	−2.270
1300	84.119	310.161	243.735	86.353	−201.620	73.410	−2.950
1400	84.119	316.395	248.706	94.765	−199.174	94.474	−3.525
1500	84.119	322.199	253 414	103.177	−196.768	115.364	−4.017

PREVIOUS: CURRENT: March 1962

$S°(298.15\ K)$ = [215.663] $J·K^{-1}·mol^{-1}$
T_{fus} = 530 K

$\Delta_f H°(298.15\ K)$ = [−87.287] $kJ·mol^{-1}$
$\Delta_{fus}H°$ = 18.966 ± 0.21 $kJ·mol^{-1}$

Enthalpy of Formation

$\Delta_f H°(HgI_2, l, 298.15\ K)$ is calculated from $\Delta_f H°(HgI_2, cr, 298.15\ K)$ by adding the enthalpy of fusion, $\Delta_{fus}H°$, and the difference in enthalpy, $H°(530\ K) H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

Heat capacity measurements were obtained from the data of Guinchant[1] in the range 540–600 K and were assumed constant above and below this range. A glass type transition is assumed at 353 K below which the heat capacity is assumed to be that of HgI_2(cr). $S°$(l, 298.15 K) is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion and Vaporization Data

T_{vap} = 627 K (1 atm) is taken from NBS,[2] $\Delta_{vap}H°$ = 14.141 ± 0.25 $kcal·mol^{-1}$ (for T_{vap} = 627 K) was obtained from the data of Prideaux[3] and Johnson.[4]

References

[1]M. Guinchant, Compt. Rend. 68, 145 (1907).
[2]U. S. Nat. Bur. Stand. Circ. 500, 1268 pp. (1952).
[3]E. B. R. Prideaux, J. Chem. Soc. (London) 97, 2032 (1910).
[4]F. M. G. Johnson, J. Amer. Chem. Soc. 33, 777 (1911).

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	77.747	215.663	215.663	0.	−87.287	−94.291	16.519
300	77.822	216.144	215.665	0.144	−87.295	−94.335	16.425
353.000	80.040	228.980	216.722	4.327	GLASS <--> LIQUID TRANSITION		
353.000	102 .090	228.980	216.722	4.327			
400	102.090	241.741	218.928	9.125	−102.717	−96.125	12.553
500	102.090	264.522	225.853	19.334	−143.432	−90.609	9.466
530.000	102 .090	270.471	228.212	22.397	----- II <--> LIQUID -----		
600	102.090	283.135	233.896	29.543	−139.692	−80.396	6.999
700	102.090	298.872	242.083	39.752	−194.724	−64.237	4.793
800	102.090	312.504	250.053	49.961	−190.373	−45.893	2.997
900	102.090	324.529	257.673	60.170	−186.033	−28.094	1.631
1000	102.090	335.285	264.906	70.379	−181.704	−10.778	0.563
1100	102.090	345.015	271.753	80.588	−177.389	6.106	−0.290
1200	102.090	353.898	278.234	90.797	−173.091	22.597	−0.984
1300	102.090	362.070	284.373	101.006	−168.817	38.731	−1.556
1400	102.090	369.635	290.196	111.215	−164.574	54.537	−2.035
1500	102.090	376.679	295.729	121.424	−160.371	70.041	−2.439

PREVIOUS CURRENT March 1962

0	to	402 K	crystal, I
402	to	530 K	crystal, II
above		530 K	liquid

Refer to the individual tables for details.

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

	$J \cdot K^{-1} mol^{-1}$			$kJ \cdot mol^{-1}$			
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							
100							
200							
250							
298.15	77.747	181.326	181.326	0.	−105.437	−102.204	17.906
300	77.822	181.807	181.328	0.144	−105.445	−102.184	17.792
400	82.006	204.768	184.430	8.135	−121.858	−100.476	13.121
402.000	82.090	205.178	184.532	8.299	I <- -> II TRANSITION		
402.000	84.119	211.433	184.532	10.814			
500	84.119	229.784	191.669	19.058	−161.859	−91.667	9.576
530.000	84.119	234.686	193.966	21.581	II <- -> LIQUID TRANSITION		
530.000	102.090	270.471	193.966	40.547			
600	102.090	283.135	203.646	47.694	−139.692	−80.396	6.999
700	102.090	298.872	216.154	57.903	−194.724	−64.237	4.793
800	102.090	312.504	227.365	68.112	−190.373	−45.893	2.997
900	102.090	324.529	237.506	78.321	−186.033	−28.094	1.631
1000	102.090	335.285	246.756	88.529	−181.704	−10.778	0.563
1100	102.090	345.015	255.253	98.738	−177.389	6.106	−0.290
1200	102.090	353.898	263.109	108.947	−173.091	22.597	−0.984
1300	102.090	362.070	270.411	119.156	−168.817	38.731	−1.556
1400	102.090	369.635	277.232	129.365	−164.574	54.537	−2.035
1500	102.090	376.679	283.629	139.574	−160.371	70.041	−2.439

PREVIOUS: CURRENT: March 1962

$S°(298.15\ K) = 336.206\ J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K) = -9.84\ kJ·mol^{-1}$

$\Delta_f H°(298.15\ K) = -16.13 \pm 2.1\ kJ·mol^{-1}$

Vibrational Frequencies and Degeneracies ν, cm^{-1}
156 (1)
33 (2)
[233](1)

Point Group: $D_{\infty h}$ $\sigma = 2$
Bond Distance: Hg–I = 2.58 Å
Bond Angle: I–Hg–I = 180°
Rotational Constant: $B_0 = 0.009978\ cm^{-1}$

Enthalpy of Formation

The enthalpy of formation of the crystal as given in National Bureau of Standards[1] was combined with the 3rd law heat of sublimation at 298.15 K derived from the data of Niwa and Shibata,[2] Magee[3] and Johnson.[4]

Heat Capacity and Entropy

The vibrational constants were given by Klemperer and Lindeman.[5] The anti-symmetric stretching frequency is estimated by analogy with the bromide and chloride. The bond length is an average of the values given by Braune and Knoke,[6] Gregg *et al*[7] and Akishin *et al*.[8]

References

[1] U. S. Nat. Bur. Stand. Circ. 500, 1268 pp. (1952).
[2] K. Niwa and Z. Shibata, J. Fac. Sci. Hokkaido Imp. Univ. Ser. III 2, 183 (1938).
[3] D. W. Magee, Univ. Microfilms No. 14474 Ann Arbor, Michigan.
[4] F. M. G. Johnson, J. Amer. Chem. Soc. 33, 777 (1911).
[5] W. Klemperer and L. Lindeman, J. Chem. Phys. 25, 397 (1956).
[6] H. Braune and S. Knoke, Naturwiss. 21, 349 (1933).
[7] A. H. Gregg, G. C. Hampson, G. I. Jenkins, P. L. F. Jones and L. E. Sutton, Trans. Faraday Soc. 33, 852 (1937).
[8] P. A. Akishin, V. P. Spiridinov and A. N. Khodchenkov, Zhur. Fiz. Khim. 33, 20 (1959).

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	−16.253	−9.841	−9.841	INFINITE
100	54.486	272.205	389.418	−11.721	−10.065	−27.465	14.346
200	59.759	312.043	341 763	−5 944	−11.805	−44.218	11.549
250	60.630	325.481	337.210	−2.932	−15.118	−52.052	10.876
298.15	61.118	336.206	336.206	0.	−16.129	−59.074	10.349
300	61.132	336.584	336.207	0.113	−16.169	−59.340	10.332
350	61.446	346.033	336.952	3.178	−17.305	−66.448	9.917
400	61.654	354.252	338.612	6.256	−34.430	−72.842	9.512
450	61.798	361.523	340.762	9.342	−36.743	−77.504	8.996
500	61.903	368.040	343.169	12.435	−79.175	−78.110	8.160
600	62.040	379.339	348.284	18.633	−79.445	−77.872	6.779
700	62.124	388.909	353.422	24.841	−138.478	−71.017	5.299
800	62.178	397.209	358.388	31.057	−138.120	−61.404	4.009
900	62.216	404.534	363.116	37.276	−137.769	−51.836	3.008
1000	62.243	411.091	367.592	43.499	−137.427	−42.306	2.210
1100	62.263	417.024	371.820	49.725	−137.095	−32.810	1.558
1200	62.278	422.443	375.816	55.952	−136.780	−23.344	1.016
1300	62.290	427.428	379.597	62.180	−136.486	−13.903	0.559
1400	62.299	432.044	383.180	68.410	−136.222	−4.484	0.167
1500	62.307	436.343	386.583	74.640	−135.997	4.918	−0 171
1600	62.313	440.364	389.820	80.871	−135.822	14.307	−0.467
1700	62.318	444.142	392.905	87.103	−135.705	23.686	−0.728
1800	62.322	447 704	395.852	93.335	−135.652	33.060	−0.959
1900	62.326	451 074	398.670	99.567	−135.669	42.433	−1.167
2000	62.329	454.271	401.371	105.800	−135.755	51.808	−1.353
2100	62.332	457.312	403.963	112.033	−135.909	61.190	−1.522
2200	62.334	460.212	406.454	118.266	−136.124	70.580	−1.676
2300	62.336	462.983	408.852	124.500	−136.395	79.982	−1.816
2400	62.338	465.636	411.164	130.733	−136.710	89.396	−1.946
2500	62.340	468.181	413.394	136.967	−137.058	98.824	−2.065
2600	62.341	470.626	415.548	143.201	−137.429	108.267	−2.175
2700	62.342	472.978	417.632	149.435	−137.811	117.724	−2.278
2800	62.343	475.246	419.649	155.670	−138.191	127.195	−2.373
2900	62.344	477.433	421.604	161.904	−138.560	136.680	−2.462
3000	62.345	479.547	423.501	168.139	−138.907	146.177	−2.545
3100	62.346	481.591	425.342	174.373	−139.225	155.685	−2.623
3200	62.347	483.571	427.131	180.608	−139.505	165.203	−2.697
3300	62.347	485.489	428.870	186.842	−139.742	174.729	−2.766
3400	62.348	487.350	430.563	193.077	−139.931	184.261	−2.831
3500	62.349	489.158	432.211	199.312	−140.067	193.799	−2.892
3600	62.349	490.914	433.818	205.547	−140.149	203.339	−2.950
3700	62.350	492.622	435.384	211.782	−140.173	212.881	−3.005
3800	62.350	494.285	436.912	218.017	−140.138	222.422	−3.057
3900	62.350	495.905	438.404	224.252	−140.044	231.962	−3.107
4000	62.351	497.483	439.862	230.487	−139.891	241.499	−3.154
4100	62.351	499.023	441.286	236.722	−139.679	251.031	−3.198
4200	62.352	500.526	442.679	242.957	−139.409	260.558	−3.241
4300	62.352	501.993	444.041	249.192	−139.082	270.077	−3.281
4400	62.352	503.426	445.374	255.428	−138.698	279.588	−3.319
4500	62.352	504.827	446.680	261.663	−138.261	289.090	−3.356
4600	62.353	506.198	447.959	267.898	−137.771	298.581	−3.390
4700	62.353	507.539	449.213	274.133	−137.230	308.061	−3.424
4800	62.353	508.852	450.441	280.369	−136.640	317.529	−3.455
4900	62.353	510.137	451.647	286.604	−136.003	326.985	−3.486
5000	62.353	511.397	452.829	292.839	−135.320	336.426	−3.515
5100	62.354	512.632	453.990	299.075	−134.595	345.854	−3.542
5200	62.354	513.842	455.129	305.310	−133.828	355.268	−3.569
5300	62.354	515.030	456.248	311.545	−133.021	364.665	−3.594
5400	62.354	516.196	457.347	317.781	−132.178	374.048	−3.618
5500	62.354	517.340	458.428	324.016	−131.298	383.414	−3.641
5600	62.354	518.463	459.490	330.252	−130.385	392.765	−3.664
5700	62.355	519.567	460.534	336.487	−129.440	402.098	−3.685
5800	62.355	520.651	461.561	342.722	−128.465	411.415	−3.705
5900	62.355	521.717	462.572	348.958	−127.462	420.715	−3.725
6000	62.355	522.765	463.567	355.193	−126.432	429.997	−3.743

PREVIOUS: March 1962 (1 atm) CURRENT: March 1962 (1 bar)

$S°(298.15\ K) = 70.270 \pm 0.13\ J \cdot K^{-1} \cdot mol^{-1}$

$\Delta_f H°(0\ K) = -86.208 \pm 0.100\ kJ \cdot mol^{-1}$
$\Delta_f H°(298.15\ K) = -90.789 \pm 0\ 100\ kJ\ mol^{-1}$

Enthalpy of Formation

Calculated from the entropy obtained by Bauer and Johnston[1] and the Gibbs energy of formation as determined from the numerous cell measurements described by Bauer and Johnston. The value adopted for $\Delta_f H°(298.15\ K)$ is $-42707 \pm 14\ cal \cdot mol^{-1}$.

Heat Capacity and Entropy

The heat capacity has been measured from 15 to 298.15 K by Bauer and Johnston.[1] The extrapolation below 15 K was done assuming a T^3 law and gave $S°(15\ K) = 0.264\ cal \cdot K^{-1} \cdot mol^{-1}$. Above 298 15 the data was extrapolated smoothly and adjusted to give the observed decomposition vapor pressures of Taylor and Hulett.[2]

Decomposition Data

According to Taylor and Hulett,[2] the vapor pressure reaches 1 89 atmospheres at 749 K This corresponds to the decomposition to 2 $Hg(g) + O_2(g)$, the equilibrium constant being unity at 1.89 atm.

References

[1]T. W. Bauer and H. L. Johnston, J. Amer. Chem. Soc. 75, 2217 (1953).
[2]G. B. Taylor and G. A. Hulett, J Phys. Chem. 17, 565 (1913).

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	−9.104	−86.208	−86.208	INFINITE
100	28.434	30.840	105.148	−7 431	−87.693	−78.390	40.947
200	38.171	53.856	74.128	−4.054	−88.357	−68.775	17.962
298.15	44.062	70.270	70.270	0.	−90.789	−58.490	10.247
300	44.145	70.543	70.271	0.082	−90.786	−58.289	10.149
400	48.325	83.836	72.055	4.712	−90.406	−47.502	6.203
500	51.631	94.990	75.556	9 717	−89.659	−36.856	3.850
600	54.120	104.632	79.617	15.009	−88.660	−26.386	2.297
700	56.066	113.127	83.809	20.523	−146.248	−9.526	0.711
800	57.509	120.711	87.956	26.204	−144.314	9.874	−0.645
900	58.626	127.553	91.982	32.013	−142.285	29.027	−1.685
1000	59 413	133.773	95.855	37.918	−140.190	47.950	−2.505

PREVIOUS: CURRENT: June 1962

$S°(298.15\ K)$ = [239.161] $J·K^{-1}·mol^{-1}$

$\Delta_f H°(0\ K)$ = [46.514] $kJ·mol^{-1}$
$\Delta_f H°(298.15\ K)$ = [41.840] $kJ·mol^{-1}$

Electronic Level and Quantum Weight		
State	ϵ_i, cm^{-1}	g_i
$^1\Sigma$	0	1

ω_e = [680] cm^{-1} $\omega_e x_e$ = [4.7] cm^{-1} σ = 1
B_e = [0.336] cm^{-1} α_e = [0.0027] cm^{-1} r_e = [1.84] Å

Enthalpy of Formation

The enthalpy of formation, $\Delta_f H°$(HgO, g, 298 15 K), is estimated to be 10 ± 15 kcal·mol^{-1} This value is obtained from the enthalpy of formation of PbO(g) and comparison of the enthalpy of formation of analogous lead and mercury compounds using the method of Karapet'yants.[1] The corresponding dissociation energy, $D_0°$(HgO,g) is 64 ± 15 kcal·mol^{-1}.

Heat Capacity and Entropy

The equilibrium internuclear separation (r_e) of HgO(g) is estimated from the corresponding quantity for PbO(g) and comparison of Hg–X and Pb–X bond distances for cases in which values of both distances are known The rotational constant B_e is calculated from r_e. The fundamental vibrational frequency ω_e is estimated from Guggenheimer's relation for multiple bonded molecules.[2] The anharmonic vibrational term $\omega_e x_e$ is calculated from $\omega_e x_e = \omega_e^2/(4D_0 + 2\ \omega_e)$. The value of α_e is calculated from the Morse potential function. The ground state configuration is estimated from the building-up principle,[3] the united atom theory,[3] and from analogy with BeO.

References

[1] M. Kh. Karapet'yants, Russ. J. Inorg. Chem. 10, 837 (1965).
[2] K. M. Guggenheimer, Proc. Phys. Soc. (London) 58, 456 (1946).
[3] G Herzberg, "Spectra of Diatomic Molecules," D. Van Nostrand Co., Inc., New York, (1950).

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

	$J·K^{-1}·mol^{-1}$			$kJ·mol^{-1}$			
T/K	$C_p°$	$S°$	$-[G°-H°(T_r)]/T$	$H°-H°(T_r)$	$\Delta_f H°$	$\Delta_f G°$	log K_f
0	0.	0.	INFINITE	−9.010	46.514	46.514	INFINITE
100	29.158	205.913	266.918	−6.101	46.266	38.062	−19.882
200	30.709	226.480	242.102	−3.124	45.202	30.259	−7.903
250	31.874	233.459	239.697	−1.560	42.341	26.742	−5.587
298.15	32.883	239.161	239.161	0.	41.840	23.784	−4.167
300	32.918	239.365	239.162	0.061	41.822	23.672	−4.122
350	33.776	244.506	239.566	1.729	41.362	20.684	−3.087
400	34.460	249.063	240.474	3.436	40.945	17.759	−2.319
450	35.002	253.154	241.659	5.173	40.557	14.884	−1.728
500	35.435	256.865	242.997	6.934	40.187	12.052	−1.259
600	36.068	263.385	245.867	10.511	39.470	6.492	−0.565
700	36.501	268.980	248.778	14.141	−20.001	7 624	−0.569
800	36.811	273.875	251.616	17.807	−20.082	11.575	−0.756
900	37.045	278.225	254.335	21.501	−20.170	15.538	−0.902
1000	37.229	282.138	256.923	25.215	−20.265	19.510	−1.019
1100	37.379	285.693	259.380	28.945	−20.368	23.493	−1.116
1200	37.504	288.951	261.710	32.690	−20.476	27.485	−1.196
1300	37.613	291.958	263.923	36.446	−20.591	31.486	−1.265
1400	37.708	294 749	266.026	40.212	−20.710	35.496	−1.324
1500	37.794	297.353	268.029	43.987	−20.834	39.515	−1.376
1600	37.873	299.795	269.938	47.770	−20.963	43.543	−1.422
1700	37.946	302.093	271.763	51.561	−21.096	47.579	−1.462
1800	38.014	304.264	273.509	55.359	−21.235	51.622	−1.498
1900	38 079	306.321	275.182	59 164	−21.378	55.674	−1.531
2000	38.141	308.276	276.788	62.975	−21.527	59.733	−1.560
2100	38.201	310.138	278.333	66.792	−21.681	63.800	−1.587
2200	38.258	311.917	279.819	70.615	−21.841	67.874	−1.612
2300	38.314	313.619	281.252	74.444	−22.006	71.956	−1.634
2400	38.369	315.250	282.635	78.278	−22.177	76.044	−1.655
2500	38.422	316.818	283.971	82.117	−22.354	80.141	−1.674
2600	38.474	318.326	285.263	85.962	−22.536	84.244	−1.692
2700	38.526	319.779	286.515	89.812	−22.723	88.355	−1.709
2800	38.577	321.181	287.728	93.667	−22.915	92 472	−1.725
2900	38.627	322.535	288.905	97.528	−23.113	96.596	−1.740
3000	38.676	323.846	290.048	101.393	−23.315	100.728	−1.754
3100	38.725	325.115	291.159	105.263	−23.521	104.866	−1.767
3200	38.774	326.345	292.239	109.138	−23.731	109.011	−1.779
3300	38.822	327.539	293.291	113.018	−23.946	113.162	−1 791
3400	38.870	328.698	294.315	116.902	−24.164	117.320	−1.802
3500	38.918	329.826	295.314	120.792	−24.385	121.485	−1.813
3600	38.965	330.923	296.288	124.686	−24.609	125.656	−1.823
3700	39.013	331.991	297.239	128.585	−24.836	129.832	−1.833
3800	39.060	333.032	298.167	132.488	−25.066	134.016	−1.842
3900	39.106	334.047	299.074	136.397	−25.297	138.206	−1.851
4000	39 153	335.038	299.961	140.310	−25.531	142.401	−1.860
4100	39.199	336.005	300.828	144.227	−25.767	146.602	−1.868
4200	39.246	336 951	301.677	148.150	−26.005	150.809	−1.876
4300	39.292	337.875	302.508	152.076	−26.245	155.022	−1.883
4400	39.338	338.778	303.322	156.008	−26.487	159.240	−1.890
4500	39.384	339 663	304.120	159 944	−26.731	163.464	−1.897
4600	39.430	340.529	304.902	163.885	−26.977	167.693	−1.904
4700	39.476	341.378	305.669	167.830	−27.226	171.927	−1.911
4800	39.521	342.209	306.422	171.780	−27.477	176.167	−1.917
4900	39.567	343.025	307.160	175.734	−27 731	180 413	−1.923
5000	39.613	343.824	307.886	179.693	−27.988	184.663	−1.929
5100	39.658	344.609	308.598	183.657	−28.249	188.919	−1.935
5200	39.704	345.380	309.298	187.625	−28.514	193.179	−1.941
5300	39.749	346.137	309.986	191.598	−28.784	197.446	−1.946
5400	39.794	346.880	310.662	195.575	−29.060	201.717	−1.951
5500	39.840	347.611	311.328	199.556	−29.342	205.993	−1.956
5600	39.885	348.329	311.982	203.543	−29.631	210.275	−1 961
5700	39.930	349.035	312.626	207.533	−29.927	214.561	−1.966
5800	39 975	349.730	313.260	211.529	−30.232	218.853	−1.971
5900	40.021	350 414	313.883	215.529	−30.547	223.150	−1.976
6000	40.066	351.087	314.498	219.533	−30.872	227.453	−1.980

PREVIOUS: June 1967 (1 atm) CURRENT: June 1967 (1 bar)

$S°(298.15\ K) = 241.29 \pm 8.4\ J·K^{-1}·mol^{-1}$
$T_{fus} = 563\ K$

$\Delta_f H°(298.15\ K) = -119.085 \pm 2.1\ kJ·mol^{-1}$
$\Delta_{fus} H° = [27.196 \pm 8.4]\ kJ·mol^{-1}$

Enthalpy of Formation

The average value of the cell measurements of Vosburgh,[1] Cohen,[2] Yoshida,[3] Oholm[4] and the calorimetric values of Varet[5] and Nernst[6] is adopted.

Heat Capacity and Entropy

The heat capacity at 298.15 K is taken from NBS[7] and is estimated above this by analogy with mercurous chloride. The entropy is obtained from the enthalpy and Gibbs energy of formation obtained from the cell measurements listed under enthalpy of formation.

Fusion Data

Yvon[8] gives 563 K for the melting point. The enthalpy of melting is estimated by assuming the entropy of melting per atom to be the same as that for mercuric iodide.

References

[1]W. C. Vosburgh, J. Amer. Chem. Soc. **50**, 2386 (1928).
[2]E. Cohen, Zeits. physik. Chem. **94**, 210 (1920).
[3]T. Yoshida, J. Chem. Soc. Japan **48**, 435 (1927).
[4]L. W. Oholm, Acta. Soc. Scientarum Fennicae **41**, 1 (1913).
[5]R. Varet, Ann. Chim. Phys. (7) **8**, 91 (1896).
[6]W. Nernst, Zeits. physik. Chem. **2**, 23 (1888).
[7]U. S. Nat. Bur. Stand. Circ. 500, 1268 pp. (1952).
[8]P. Yvon, Comp. Rend. **76**, 1607 (1873).

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							
100							
200							
250							
298.15	105.855	241.291	241.291	0.	−119.085	−111.063	19.458
300	105.868	241.946	241.293	0.196	−119.093	−111.013	19.329
400	110.416	273.066	245.506	11.024	−135.435	−107.707	14.065
500	113 679	298.073	253.599	22.237	−177.873	−96.702	10.102
563.000	115 .244	311.658	259.349	29.450	--- CRYSTAL <---> LIQUID ---		
600	116.064	319.018	262.804	33.729	−175.564	−80.680	7.024
700	117.905	337.052	272.152	45.430	−290.578	−51.920	3.874
800	119.411	352.898	281.275	57.298	−286.646	−18.092	1.181
900	120.625	367.034	290.033	69.301	−282.590	15.235	−0.884
1000	121.713	379.800	298.381	81.419	−278.432	48.104	−2.513
1100	122.687	391.447	306.320	93.640	−274.183	80.553	−3.825
1200	123.554	402.161	313.866	105.953	−269.860	112.611	−4.902
1300	124.236	412.076	321.044	118.341	−265.485	144.307	−5.798
1400	125.143	421.314	327.880	130.808	−261.062	175.664	−6.554
1500	126.273	429.986	334.401	143.377	−256.578	206.702	−7.198

PREVIOUS. CURRENT March 1962

$S°$(298.15 K) = [273.258] J·K^{-1}·mol^{-1}
T_{fus} = 563 K

$\Delta_f H°$(298.15 K) = [−98.564] kJ·mol^{-1}
$\Delta_{fus} H°$ = [27 196 ± 8.4] kJ·mol^{-1}

Enthalpy of Formation

$\Delta_f H°(Hg_2I_2, l, 298.15\ K)$ is calculated from $\Delta_f H°(Hg_2I_2, cr, 298.15\ K)$ by adding the enthalpy of fusion, $\Delta_{fus} H°$, and the difference in enthalpy, $H°(563\ K) - H°(298.15\ K)$, between the crystal and liquid.

Heat Capacity and Entropy

$C_p°$ is estimated as 1.33 times the heat capacity of mercuric iodide $S°(l, 298.15\ K)$ is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

The melting point was given by Yvon.[1] The enthalpy of melting was estimated from that of mercuric iodide, by assuming the entropies of melting per atom to be equal.

Vaporization Data

Mercurous iodide decomposes to Hg(g) and HgI_2(g) at the boiling point which was estimated from the Gibbs energy change of the reaction. For 1 atm, T_{vap} = [630] K (decomposition).

Reference

[1]P. Yvon, Comp. Rend. 76, 1607 (1873).

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	136.398	273.258	273.258	0.	−98.564	−100.073	17.532
300	136.398	274.101	273.260	0.252	−98.516	−100.082	17.426
400	136.398	313.341	278.610	13.892	−112.046	−100.428	13.115
500	136.398	343.777	288.713	27.532	−152.057	−93.738	9.793
563.000	136.398	359.964	295.798	36.125	--- CRYSTAL <--> LIQUID ---		
600	136.398	368.646	300.026	41.172	−147.600	−82.493	7.182
700	136.398	389.672	311.369	54.812	−260.675	−58.850	4.391
800	136.398	407.885	322.321	68.452	−254.971	−30.408	1.985
900	136.398	423.950	332.738	82.091	−249.279	−2.679	0.155
1000	136.398	438.321	342.590	95.731	−243.598	24.416	−1.275
1100	136.398	451.322	351.893	109.371	−237.931	50.943	−2.419
1200	136.398	463.190	360.681	123.011	−232.281	76.955	−3.350
1300	136.398	474.107	368.992	136.651	−226.654	102.496	−4.118
1400	136.398	484.216	376.865	150.291	−221.059	127.605	−4.761
1500	136.398	493.626	384.339	163.930	−215.503	152.316	−5.304

PREVIOUS: CURRENT: March 1962

0	to	563 K	crystal
above		563 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^{-1}mol^{-1}			kJ·mol^{-1}			
0							
100							
200							
250							
298.15	105.855	241.291	241.291	0	−119.085	−111.063	19.458
300	105.868	241.946	241.293	0.196	−119.093	−111.013	19.329
400	110.416	273.066	245.506	11.024	−135.435	−107.707	14.065
500	113.679	298.073	253.599	22.237	−177.873	−96.702	10.102
563.000	115.244	311.658	259.349	29.450	CRYSTAL <--> LIQUID TRANSITION		
563.000	136.398	359.964	259.349	56.646			
600	136.398	368.646	265.824	61.693	−147.600	−82.493	7.182
700	136.398	389.672	282.053	75.333	−260.675	−58.850	4.391
800	136.398	407.885	296.669	88.972	−254.971	−30.408	1.985
900	136.398	423.950	309.937	102.612	−249.279	−2.679	0.155
1000	136.398	438.321	322.069	116.252	−243.598	24.416	−1.275
1100	136.398	451.322	333.238	129.892	−237.931	50.943	−2.419
1200	136.398	463.190	343.580	143.532	−232.281	76.955	−3.350
1300	136.398	474.107	353.206	157.172	−226.654	102.496	−4.118
1400	136.398	484.216	362.207	170.811	−221.059	127.605	−4.761
1500	136.398	493.626	370.659	184.451	−215.503	152.316	−5.304

PREVIOUS: CURRENT: March 1962