

Iodine (I)

IDEAL GAS

$A_1 = 126.9045$  Iodine (I)

I<sub>2</sub>(g)

IP(I, g) = 84295.1 ± 0.2 cm<sup>-1</sup>  
 $S^{\circ}(298.15 \text{ K}) = 180.786 \pm 0.002 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$

$\Delta_f H^{\circ}(0 \text{ K}) = 107.16 \pm 0.04 \text{ kJ} \cdot \text{mol}^{-1}$   
 $\Delta_f H^{\circ}(298.15 \text{ K}) = 106.76 \pm 0.04 \text{ kJ} \cdot \text{mol}^{-1}$

Electronic Levels and Quantum Weights	$\epsilon$ , cm <sup>-1</sup>	g
State		
<sup>2</sup> P <sub>1/2</sub>	0.0	4
<sup>2</sup> P <sub>3/2</sub>	7603.15	2

Enthalpy of Formation

The adopted value for the enthalpy of formation of I(g) is derived from the spectroscopically determined dissociation energy of I<sub>2</sub>(g) as reported by Barrow *et al.*<sup>12</sup> This value is also recommended by Brewer and Winn<sup>3</sup> and Huber and Herzberg.<sup>4</sup> The adopted value is  $D_0(\text{I}_2, \text{g}) = 12440.06 \pm 0.03 \text{ cm}^{-1}$  (148.816 ± 0.001 kJ·mol<sup>-1</sup>). The convergence limit in the absorption spectrum of the <sup>1</sup>I<sub>0<sub>v</sub></sub> - <sup>2</sup>Σ<sub>g</sub> system corresponds to dissociation to a ground state iodine atom (<sup>2</sup>P<sub>1/2</sub>) and an excited state iodine atom (<sup>2</sup>P<sub>3/2</sub>).

Using earlier data, the CODATA recommended value<sup>5</sup> was calculated using  $D_0(\text{I}_2, \text{g}) = 12440.9 \pm 1.1 \text{ cm}^{-1}$  from LeRoy,<sup>6</sup> Brown,<sup>7</sup> LeRoy and Bernstein,<sup>8</sup> and Sitterley.<sup>9</sup> LeRoy,<sup>7</sup> LeRoy and Bernstein,<sup>8</sup> and a recent study by LeRoy and Bernstein<sup>10</sup> obtained the dissociation energy from the analysis of the distribution of the uppermost vibrational levels. Their calculations were based on the data of Brown,<sup>7</sup> with reference to the study by Verma.<sup>11</sup>

Heat Capacity and Entropy

Information on the electronic energy levels and quantum weights is taken from Moore.<sup>12,13</sup> Only two levels are included in the calculation. All other levels (observed and predicted) lie above 54633 cm<sup>-1</sup>. Our calculations indicate that any reasonable method of filling in the missing levels and cutting off the summation in the partition function<sup>14</sup> has no effect on the thermodynamic properties to 6000 K. This is undoubtedly a result of the high energy of these levels. Therefore, we list only the ground state and the first excited state. Extension to higher temperatures may require consideration of the higher excited states and utilization of different fill and cutoff procedures.

The thermodynamic functions at 298.15 K are in agreement with recent CODATA recommendations<sup>15</sup> except for two minor differences. First, the entropy differs by 0.1094 J·K<sup>-1</sup>·mol<sup>-1</sup> because this table uses a standard-state pressure of 1 bar, whereas the CODATA recommendations are based on 1 atm. Second, entropy differences of the order of 0.001–0.004 J·K<sup>-1</sup>·mol<sup>-1</sup> for the monatomic halogens arise due to the use of slightly different values for the relative atomic mass and for R; in this table uses 8.31441 J·K<sup>-1</sup>·mol<sup>-1</sup>. Considering these minor changes, this table agrees within the estimated uncertainty with those by Hultgren *et al.*,<sup>16</sup> Gurvich *et al.*,<sup>17</sup> and Wagman *et al.*<sup>18</sup> The estimated uncertainty is due to uncertainties in the relative atomic mass and fundamental constants which are based on the 1981 scale<sup>18</sup> and the 1973 values,<sup>19</sup> respectively.

References

1. R. F. Barrow, D. F. Broyd, L. B. Pederson and K. K. Yee, *Chem. Phys. Letters* **18**, 357 (1973).
2. R. F. Barrow, Clark, Coxon and K. K. Yee, *J. Mol. Spectrosc.* **51**, 428 (1974).
3. L. Brewer and J. S. Winn, *Faraday Symp. Chem. Soc. (GB)* **14**, 126 (1980).
4. K. P. Huber and G. Herzberg, "Constants of Diatomic Molecules," Van Nostrand Reinhold Company, New York, N.Y. (1979).
5. J. D. Cox, *J. Chem. Thermodyn.* **4**, 331 (1972).
6. R. J. LeRoy, *J. Chem. Phys.* **52**, 2678 (1970).
7. W. G. Brown, *Phys. Rev.* **38**, 709 (1931).
8. R. J. LeRoy and R. B. Bernstein, *J. Chem. Phys.* **52**, 3869 (1970).
9. C. M. Sitterley, *U. S. Nat. Bur. Stand., personal communication to ISCU-CODATA Task Group on Key Values for Thermodynamics.*
10. R. J. LeRoy and R. B. Bernstein, *Chem. Phys. Lett.* **5**, 42 (1970); *J. Mol. Spectrosc.* **37**, 109 (1971).
11. R. D. Varma, *J. Chem. Phys.* **32**, 738 (1960).
12. C. E. Moore, *U. S. Nat. Bur. Stand., NSRDS-NBS-34*, (1970).
13. C. E. Moore, *U. S. Nat. Bur. Stand., NSRDS-NBS-35*, Vol. II, 1970 [Reprint of NBS Circular 467, Volume II, 1952].
14. J. D. Cox, chairman, ISCU-CODATA Task Group on Key Values for Thermodynamics, *J. Chem. Thermodyn.*, **10**, 903 (1978).
15. R. Hultgren, P. D. Desai *et al.*, "Selected Values of the Thermodynamic Properties of the Elements," American Society for Metals, Metals Park, Ohio, (1973).
16. L. V. Gurvich, I. V. Veits *et al.*, "Thermodynamic Properties of Individual Substances," 3rd ed., Vol. I, Nauka, Moscow, (1978).
17. N. E. Holden and R. L. Martin, *Pure App. Chem.* **55**, 1101 (1983).
18. E. R. Cohen and B. N. Taylor, *J. Phys. Chem. Ref. Data* **2**, 663 (1973).
19. D. D. Wayne, W. H. Evans *et al.*, *J. Phys. Chem. Ref. Data* **11**, Supp. 2 (1982).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>f</sub> H <sup>o</sup>	
0	0	INFINITE	0	107.164	INFINITE
100	20.786	158.079	-6.197	107.164	99.559
200	20.787	182.688	-2.040	107.330	-49.601
250	20.786	177.125	-1.001	107.055	-15.502
298.15	20.786	180.786	0.	106.762	76.109
300	20.786	180.915	0.038	106.750	-12.294
350	20.786	184.119	1.078	106.383	69.947
400	20.786	186.595	1.816	105.804	-12.179
450	20.786	189.343	2.329	105.010	-9.578
500	20.786	191.533	2.656	104.032	-7.582
600	20.786	195.323	3.424	102.905	-5.167
700	20.786	198.577	4.166	101.590	-3.245
800	20.787	201.302	4.832	100.141	-1.791
900	20.789	203.571	5.352	98.510	-0.884
1000	20.795	205.942	5.752	96.759	-0.325
1100	20.806	207.924	6.069	94.937	0.090
1200	20.824	209.735	6.310	93.084	0.259
1300	20.851	211.403	6.485	91.215	0.409
1400	20.889	212.949	6.597	89.333	0.542
1500	20.936	214.392	6.646	87.442	0.661
1600	20.994	215.745	6.632	85.546	0.768
1700	21.062	217.020	6.559	83.648	0.865
1800	21.137	218.226	6.424	81.745	0.953
1900	21.220	219.371	6.232	79.832	1.034
2000	21.308	220.461	5.986	77.911	1.107
2100	21.399	221.503	5.690	76.000	1.175
2200	21.493	222.504	5.346	74.100	1.237
2300	21.588	223.458	4.954	72.215	1.295
2400	21.682	224.379	4.514	70.342	1.349
2500	21.775	225.266	4.030	68.480	1.398
2600	21.865	226.122	3.504	66.630	1.445
2700	21.953	226.949	2.938	64.790	1.489
2800	22.036	227.749	2.332	62.960	1.529
2900	22.116	228.523	1.686	61.140	1.568
3000	22.191	229.274	1.000	59.330	1.604
3100	22.261	230.003	0.274	57.530	1.638
3200	22.327	230.711	-0.492	55.740	1.670
3300	22.387	231.399	-1.216	53.960	1.700
3400	22.443	232.068	-1.898	52.190	1.729
3500	22.494	232.720	-2.540	50.430	1.757
3600	22.540	233.354	-3.142	48.680	1.783
3700	22.581	233.972	-3.704	46.940	1.808
3800	22.618	234.575	-4.226	45.210	1.832
3900	22.651	235.163	-4.708	43.490	1.855
4000	22.679	235.736	-5.150	41.780	1.877
4100	22.704	236.297	-5.552	40.080	1.898
4200	22.725	236.844	-5.914	38.390	1.919
4300	22.743	237.379	-6.236	36.710	1.938
4400	22.757	237.902	-6.518	35.040	1.957
4500	22.769	238.414	-6.760	33.380	1.976
4600	22.777	238.914	-6.962	31.730	1.993
4700	22.783	239.404	-7.124	30.090	2.010
4800	22.787	239.884	-7.256	28.460	2.027
4900	22.788	240.354	-7.358	26.840	2.043
5000	22.787	240.814	-7.430	25.230	2.058
5100	22.784	241.265	-7.472	23.630	2.073
5200	22.780	241.708	-7.485	22.040	2.088
5300	22.774	242.142	-7.468	20.460	2.102
5400	22.766	242.567	-7.422	18.890	2.116
5500	22.757	242.985	-7.346	17.330	2.129
5600	22.747	243.395	-7.230	15.780	2.143
5700	22.736	243.797	-7.074	14.240	2.157
5800	22.724	244.193	-6.878	12.710	2.171
5900	22.711	244.581	-6.642	11.190	2.185
6000	22.697	244.963	-6.366	9.680	2.199

PREVIOUS: June 1974 (1 atm)

CURRENT: June 1982 (1 bar)

Iodine (I)

I<sub>2</sub>(g)

Iodine, Ion (I<sup>+</sup>)

IP(I<sup>+</sup>, g, 0 K) = 154304 ± 1 cm<sup>-1</sup>  
 S<sup>o</sup>(298.15 K) = 182.642 ± 0.005 J·K<sup>-1</sup>·mol<sup>-1</sup>

Iodine, Ion (I<sup>-</sup>)

M<sub>r</sub> = 126.90395

ΔH<sup>o</sup>(0 K) = 1115.557 ± 0.05 kJ·mol<sup>-1</sup>  
 ΔH<sup>o</sup>(298.15 K) = [1121.353] kJ·mol<sup>-1</sup>

I<sub>2</sub>(g)

Standard State Pressure = p<sup>o</sup> = 0.1 MPa

Electronic Levels and Quantum Weights	g <sub>e</sub>
State	cm <sup>-1</sup>
3P	0.0
1P <sub>1</sub>	7087.0
1P <sub>0</sub>	6447.9
1D <sub>2</sub>	13731
1S <sub>0</sub>	32629

## Enthalpy of Formation

ΔH<sup>o</sup>(I<sup>+</sup>, g, 0 K) is calculated from ΔH<sup>o</sup>(I, g, 0 K) using the spectroscopic value of IP(0) = 84295.1 ± 0.2 cm<sup>-1</sup> (1008.39 ± 0.01 kJ·mol<sup>-1</sup>) from Moore.<sup>2</sup> The ionization limit is converted from cm<sup>-1</sup> to kJ·mol<sup>-1</sup> using the factor, 1 cm<sup>-1</sup> = 0.01196266 kJ·mol<sup>-1</sup>, which is derived from the 1973 CODATA fundamental constants.<sup>3</sup> Rosenstock *et al.*<sup>4</sup> and Levin and Lias<sup>5</sup> have summarized additional ionization potential and appearance potential data.

ΔH<sup>o</sup>(I<sup>-</sup>, g, 298.15 K) is calculated from ΔH<sup>o</sup>(I, g, 0 K) by using IP(0) with JANAF<sup>1</sup> enthalpies, H<sup>o</sup>(0 K) - H<sup>o</sup>(298.15 K), for I(g), I<sup>+</sup>(g), and e<sup>-</sup>(ref). ΔH<sup>o</sup>(I → I<sup>+</sup> + e<sup>-</sup>, 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.*<sup>4</sup> ΔH<sup>o</sup>(298.15 K) should be changed by -6.197 kJ·mol<sup>-1</sup> 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,<sup>2,6</sup> 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<sup>7</sup> 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 lowest four excited states; the next lowest level is approximately 81040 cm<sup>-1</sup> above the ground state. Since inclusion of these upper levels has no effect on the thermodynamic functions (to 6000 K), we list only the ground state and four excited states, with the energy of these states taken from recent study by Moore.<sup>2,6</sup> The reported uncertainty in S<sup>o</sup>(298.15 K) is due to uncertainties in the relative ionic mass, fundamental constants, and the position of the four lowest excited states. Extension of these calculations above 6000 K may require consideration of the higher excited states and use of different fill and cutoff procedures.<sup>7</sup>

## References

- <sup>1</sup>JANAF Thermochemical Tables: I(g), 3-31-82; e<sup>-</sup>(ref), 3-31-82.
- <sup>2</sup>C. E. Moore, U. S. Nat. Bur. Stand., NSRDS-NBS-34, 8 pp. (1970).
- <sup>3</sup>E. R. Cohen and B. N. Taylor, J. Phys. Chem. Ref. Data 2, 663 (1973).
- <sup>4</sup>H. M. Rosenstock, K. Draxl *et al.*, J. Phys. Chem. Ref. Data 6, Supp. 1, 783 pp. (1977).
- <sup>5</sup>R. D. Levin and S. G. Lias, U. S. Nat. Bur. Stand., NSRDS-NBS-71, 634 pp. (1982).
- <sup>6</sup>C. E. Moore, U. S. Nat. Bur. Stand., NSRDS-NBS-35, Volume III, (1970) [reprint of NBS Circular 467, Volume III, 1958].
- <sup>7</sup>J. R. Downey, Jr., The Dow Chemical Company, AFOSR-TR-78-0960, Contract No. F44620-75-1-0048, (1978).

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )/T	ΔH <sup>o</sup>	ΔG <sup>o</sup>	log K <sub>r</sub>
		S <sup>o</sup> - S <sup>o</sup> (T <sub>r</sub> )/T	J·K <sup>-1</sup> ·mol <sup>-1</sup>				
0	0	INFINITE	0	-6.197	1115.557		
100	20.786	159.934	201.122	-4.119			
200	20.786	174.342	184.543	-2.040			
250	20.786	178.980	182.984	-1.001			
298.15	20.786	182.642	182.642	0	1121.353	1077.957	-188.854
300	20.786	182.770	182.642	0.038	1121.379	1077.688	-187.642
350	20.786	182.974	182.895	1.078	1122.052	1070.552	-159.741
400	20.786	188.750	183.437	2.117	1114.718	1063.195	-138.839
450	20.786	191.198	184.184	3.156	1114.780	1056.751	-122.664
500	20.786	193.588	184.997	4.196	1094.777	1052.200	-109.925
600	20.786	197.178	186.721	6.274	1097.057	1043.470	-90.842
700	20.787	200.382	188.449	8.353	1099.330	1034.359	-77.185
800	20.790	203.158	190.118	10.432	1101.598	1024.923	-66.921
900	20.800	205.607	191.706	12.511	1103.861	1015.203	-58.921
1000	20.819	207.600	193.208	14.592	1106.119	1005.231	-52.508
1100	20.852	209.785	194.626	16.675	1108.374	995.032	-47.250
1200	20.903	212.002	195.966	18.763	1110.624	984.629	-42.860
1300	20.974	213.277	197.234	20.857	1112.868	974.039	-39.137
1400	21.063	214.835	198.436	22.959	1115.105	963.276	-35.940
1500	21.176	216.292	199.578	25.070	1117.332	952.353	-33.164
1600	21.305	217.663	200.666	27.194	1119.546	941.282	-30.730
1700	21.450	218.959	201.705	29.332	1121.744	930.073	-28.578
1800	21.608	220.189	202.698	31.485	1123.925	918.735	-26.661
1900	21.776	221.362	203.649	33.654	1126.088	907.277	-24.943
2000	21.952	222.483	204.563	35.840	1128.233	895.705	-23.395
2100	22.134	223.559	205.442	38.045	1130.361	884.026	-21.989
2200	22.320	224.593	206.289	40.267	1132.477	872.246	-20.710
2300	22.506	225.589	207.107	42.509	1134.585	860.370	-19.540
2400	22.693	226.551	207.897	44.769	1136.688	848.403	-18.465
2500	22.879	227.481	208.662	47.047	1138.793	836.348	-17.475
2600	23.062	228.382	209.403	49.344	1140.906	824.208	-16.559
2700	23.241	229.256	210.122	51.659	1143.031	811.987	-15.709
2800	23.416	230.104	210.821	53.992	1145.175	799.687	-14.918
2900	23.587	230.929	211.500	56.343	1147.341	787.310	-14.181
3000	23.751	231.731	212.161	58.710	1149.535	774.838	-13.491
3100	23.910	232.513	212.805	61.093	1151.760	763.322	-12.846
3200	24.062	233.274	213.433	63.491	1154.019	751.764	-12.238
3300	24.208	234.017	214.046	65.905	1156.315	740.168	-11.662
3400	24.346	234.741	214.644	68.335	1158.649	728.532	-11.128
3500	24.478	235.449	215.228	70.774	1161.022	716.857	-10.619
3600	24.603	236.140	215.799	73.228	1163.436	705.139	-10.137
3700	24.720	236.816	216.358	75.694	1165.891	693.399	-9.680
3800	24.830	237.477	216.905	78.172	1168.387	681.653	-9.247
3900	24.933	238.123	217.441	80.660	1170.922	669.905	-8.834
4000	25.029	238.756	217.966	83.158	1173.498	658.162	-8.442
4100	25.118	239.375	218.481	85.666	1176.112	646.424	-8.068
4200	25.200	239.981	218.986	88.182	1178.764	634.691	-7.711
4300	25.276	240.575	219.481	90.705	1181.452	622.964	-7.369
4400	25.345	241.157	219.967	93.236	1184.176	611.246	-7.043
4500	25.407	241.727	220.444	95.774	1186.934	599.539	-6.730
4600	25.464	242.286	220.913	98.318	1189.725	587.843	-6.430
4700	25.514	242.834	221.373	100.867	1192.546	576.158	-6.142
4800	25.559	243.372	221.826	103.420	1195.398	564.484	-5.866
4900	25.598	243.899	222.271	105.978	1198.277	552.830	-5.600
5000	25.632	244.417	222.709	108.540	1201.184	541.167	-5.344
5100	25.661	244.925	223.140	111.104	1204.116	529.507	-5.098
5200	25.685	245.423	223.563	113.672	1207.072	483.866	-4.860
5300	25.705	245.913	223.980	116.241	1210.052	469.930	-4.631
5400	25.720	246.393	224.391	118.813	1213.052	455.937	-4.410
5500	25.732	246.865	224.795	121.385	1216.074	441.889	-4.197
5600	25.739	247.329	225.194	123.959	1219.115	427.786	-3.990
5700	25.743	247.785	225.586	126.533	1222.174	413.628	-3.790
5800	25.740	248.233	225.973	129.107	1225.249	399.416	-3.597
5900	25.740	248.673	226.354	131.682	1228.342	385.151	-3.410
6000	25.734	249.105	226.729	134.255	1231.449	370.833	-3.228

CURRENT, June 1982 (1 bar)

PREVIOUS

Iodine, Ion (I<sup>-</sup>)I<sub>2</sub>(g)

I(g)

Iodine, Ion (I<sup>+</sup>)

IDEAL GAS

Iodine, Ion (I<sup>+</sup>)

EA(I, g) = 3.0591 ± 0.0004 eV  
 S°(298.15 K) = 169.260 ± 0.005 J·K<sup>-1</sup>·mol<sup>-1</sup>  
 ΔH°(0 K) = -187.992 ± 0.4 kJ·mol<sup>-1</sup>  
 ΔH°(298.15 K) = [-194.591] kJ·mol<sup>-1</sup>

Electronic Level and Quantum State	Weight
ε <sub>n</sub> , cm <sup>-1</sup>	g <sub>n</sub>
1S <sub>0</sub>	0.0
1	1

**Enthalpy of Formation**

ΔH°(I<sup>+</sup>, g, 0 K) is calculated from ΔH°(I, g, 0 K) using the adopted electron affinity of EA (I) = 3.0591 ± 0.0004 eV (295.156 ± 0.039 kJ·mol<sup>-1</sup>). This value, recommended by Hotop and Lineberger,<sup>6</sup> is based on laser photogalvanic spectroscopy.<sup>5</sup> Additional information on I(g) may be obtained in the critical discussions of Hotop and Lineberger,<sup>6</sup> Rosenstock *et al.*,<sup>3</sup> and Massey.<sup>4</sup>

ΔH°(I<sup>+</sup>, g, 298.15 K) is obtained from ΔH°(I, g, 0 K) by using EA(I) with JANAF<sup>7</sup> enthalpies, H°(0 K) - H°(298.15 K), for I(g), I(g), and e<sup>-</sup> (ref). ΔH°(I<sup>+</sup> → I + e<sup>-</sup>, 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.*<sup>3</sup> ΔH°(298.15 K) should be changed by +6.197 kJ·mol<sup>-1</sup> if it is to be used in the ion convention that excludes the enthalpy of the electron.

**Heat Capacity and Entropy**

The ground state configuration for I<sup>+</sup>(g) is given by Hotop and Lineberger,<sup>2,6</sup> Rosenstock *et al.*,<sup>3</sup> and Massey.<sup>4</sup> Lacking any experimental evidence as to the stability of any excited states, we assume that no stable excited states exist.

The entropy at all temperatures (0-6000 K) agrees within 0.001 J·K<sup>-1</sup>·mol<sup>-1</sup> with the values of Gurvich *et al.*<sup>8</sup> except for one minor difference. The entropy differs by 0.1094 J·K<sup>-1</sup>·mol<sup>-1</sup> because this table uses a standard-state pressure of 1 bar, whereas the tabulation of Gurvich, *et al.*<sup>8</sup> is based on 1 atm. The estimated uncertainty is due to uncertainties in the relative ionic mass and the fundamental constants which are based on the 1981 scale<sup>9</sup> and the 1973 values,<sup>1</sup> respectively.

**References**

- <sup>1</sup>JANAF Thermochemical Tables: I(g), 6-30-82, e<sup>-</sup> (ref), 3-31-82.
- <sup>2</sup>H. Hotop and W. C. Lineberger, *J. Phys. Chem. Ref. Data* 4, 539 (1975).
- <sup>3</sup>H. M. Rosenstock, K. Draxl *et al.*, *J. Phys. Chem. Ref. Data* 6, Supp. 1, 783 pp. (1977).
- <sup>4</sup>H. S. W. Massey, "Negative Ions," 3rd ed., Cambridge University Press, Cambridge, 741 pp. (1976).
- <sup>5</sup>C. R. Webster, I. S. McDermaid, and C. T. Retimer, *J. Chem. Phys.* 78, 646 (1983).
- <sup>6</sup>H. Hotop and W. C. Lineberger, *J. Phys. Chem. Ref. Data* 14, 731 (1985).
- <sup>7</sup>R. C. Cohen and B. N. Taylor, *J. Phys. Chem. Ref. Data* 2, 663 (1973).
- <sup>8</sup>L. V. Gurvich, I. V. Veits *et al.*, "Thermodynamic Properties of Individual Substances", 3rd ed., Vol. 1, Nauka, Moscow, (1978).
- <sup>9</sup>N. E. Holden and R. L. Martin, *Pure Appl. Chem.* 55, 1101 (1983).

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>
		S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	ΔH°	ΔG°	
0	0	INFINITE	-6.197	-187.992		
100	20.786	146.553	-4.119			
200	20.786	160.961	-2.940			
250	20.786	165.599	-1.001			
298.15	20.786	169.260	0	-194.591	-221.488	38.804
300	20.786	169.389	0.038	-194.642	-221.654	38.593
350	20.786	172.593	1.078	-196.048	-226.047	33.736
400	20.786	175.368	2.117	-205.461	-229.961	27.030
450	20.786	177.817	3.156	-207.477	-232.902	20.447
500	20.786	180.007	4.196	-229.559	-233.720	20.404
600	20.786	183.796	6.274	-234.376	-234.717	17.515
700	20.786	187.001	8.353	-233.320	-234.717	15.330
800	20.786	189.716	10.431	-235.209	-234.788	13.617
900	20.786	192.224	12.510	-237.104	-234.621	12.236
1000	20.786	194.414	14.589	-239.005	-234.243	11.096
1100	20.786	196.396	18.244	-240.913	-233.675	10.159
1200	20.786	198.204	18.746	-242.829	-232.932	9.323
1300	20.786	199.868	18.849	-244.757	-232.029	8.618
1400	20.786	201.408	18.509	-246.701	-230.977	8.002
1500	20.786	202.842	18.6188	-248.664	-229.786	7.459
1600	20.786	204.184	18.7271	-250.653	-228.463	6.975
1700	20.786	205.444	18.8304	-252.671	-227.014	6.542
1800	20.786	206.632	18.9289	-254.721	-225.446	6.152
1900	20.786	207.756	19.0232	-256.807	-223.763	5.797
2000	20.786	208.822	19.1135	-258.927	-221.969	5.474
2100	20.786	209.836	19.2001	-261.081	-220.082	5.178
2200	20.786	210.803	19.2834	-263.266	-218.064	4.905
2300	20.786	211.727	19.3636	-265.479	-215.954	4.652
2400	20.786	212.612	19.4408	-267.714	-213.759	4.418
2500	20.786	213.461	19.5153	-269.966	-211.465	4.200
2600	20.786	214.276	19.5873	-272.229	-209.080	3.997
2700	20.786	215.060	19.6570	-274.497	-206.608	3.807
2800	20.786	215.816	19.7243	-276.765	-204.053	3.628
2900	20.786	216.546	19.7897	-279.027	-201.416	3.460
3000	20.786	217.250	19.8530	-281.279	-198.701	3.301
3100	20.786	217.932	19.9145	-283.516	-195.950	3.151
3200	20.786	218.592	19.9742	-285.734	-193.020	3.009
3300	20.786	219.231	20.0323	-287.931	-190.126	2.875
3400	20.786	219.852	20.0889	-290.103	-187.123	2.747
3500	20.786	220.454	20.1439	-292.249	-184.063	2.625
3600	20.786	221.040	20.1975	-294.368	-180.942	2.510
3700	20.786	221.610	20.2498	-296.458	-177.762	2.399
3800	20.786	222.164	20.3009	-298.519	-174.527	2.293
3900	20.786	222.704	20.3507	-300.550	-171.237	2.192
4000	20.786	223.230	20.3993	-302.551	-167.896	2.096
4100	20.786	223.743	20.4469	-304.523	-164.505	2.003
4200	20.786	224.244	20.4934	-306.466	-161.067	1.914
4300	20.786	224.733	20.5389	-308.380	-157.582	1.829
4400	20.786	225.211	20.5834	-310.265	-154.053	1.747
4500	20.786	225.678	20.6269	-312.124	-150.482	1.668
4600	20.786	226.135	20.6696	-313.956	-146.870	1.592
4700	20.786	226.582	20.7115	-315.762	-143.218	1.518
4800	20.786	227.020	20.7525	-317.543	-139.520	1.448
4900	20.786	227.448	20.7927	-319.299	-135.801	1.379
5000	20.786	227.868	20.8322	-321.033	-132.039	1.313
5100	20.786	228.280	20.8709	-322.744	-128.241	1.250
5200	20.786	228.684	20.9089	-324.434	-124.411	1.188
5300	20.786	229.079	20.9463	-326.103	-120.549	1.128
5400	20.786	229.468	20.9830	-327.752	-116.655	1.071
5500	20.786	229.849	21.0190	-329.381	-112.731	1.015
5600	20.786	230.224	21.0545	-330.993	-108.777	0.960
5700	20.786	230.592	21.0893	-332.587	-104.795	0.908
5800	20.786	230.953	21.1236	-334.164	-100.784	0.857
5900	20.786	231.309	21.1573	-335.724	-96.747	0.807
6000	20.786	231.658	21.1905	-337.269	-92.684	0.807

PREVIOUS:

CURRENT: June 1982 (1 bar)

I(g)

Iodine, Ion (I<sup>+</sup>)

## Potassium Iodide (KI)

## CRYSTAL

$$M_r = 166.0028$$

## Potassium Iodide (KI)

I<sub>1</sub>K<sub>1</sub>(cr)

$S^\circ(298.15 \text{ K}) = 106.387 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = 954 \text{ K}$   
 $\Delta H_f^\circ(0 \text{ K}) = -326.93 \pm 0.4 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta H_f^\circ(298.15 \text{ K}) = -327.90 \pm 0.4 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{sub}}H^\circ = 24.016 \text{ kJ}\cdot\text{mol}^{-1}$

## Enthalpy of Formation

The enthalpies of solution of KI(cr) have been critically reviewed by Parker.<sup>1</sup> Six pertinent results are quoted in the table below. Adopting the best value,  $\Delta_{\text{sol}}H^\circ(298.15 \text{ K}) = 4.86 \pm 0.03 \text{ kcal}\cdot\text{mol}^{-1}$ , reported by Parker, and  $\Delta H_f^\circ(298.15 \text{ K}) = -60.32$  and  $-13.19 \text{ kcal}\cdot\text{mol}^{-1}$  for K<sup>+</sup>(aq, ∞) and I<sup>-</sup>(aq, ∞), respectively, obtained from,<sup>2</sup> we obtain  $\Delta_fH^\circ(\text{KI, cr, } 298.15 \text{ K}) = -78.37 \pm 0.1 \text{ kcal}\cdot\text{mol}^{-1}$ , which is adopted.

$\Delta_fH^\circ$ , kcal·mol <sup>-1</sup> (a)	T/°C	n(b)	Source
4.830 ± 0.05	19	200	Thomsen <sup>3</sup>
4.897 ± 0.04	18	25	Wust and Lange <sup>4</sup>
4.873	25	500	Lange and Martin <sup>5</sup>
4.790 ± 0.10	20.5	600	Popov <i>et al.</i> <sup>6</sup>
5.020	24.5	18.5	Bobelsky and Lairsch <sup>7</sup>
4.830 ± 0.07	25	75000	Kapustinskii and Drakin <sup>8</sup>

a Values are adjusted to 298.15 K and to infinite dilution.

b n is the number of moles of H<sub>2</sub>O per mole of KI(cr) in solution.

## Heat Capacity and Entropy

The low temperature heat capacities are based on those measured by Berg and Morrison,<sup>9</sup> 2.86–268.0 K. The adopted values are in good agreement with the  $C_p$  values reported by Scales,<sup>10</sup> 2–7 K. The data of Clausius *et al.*,<sup>11</sup> 10.27–269.9 K, appear to be too low in the temperature range 70–270 K and are not used. Low temperature enthalpies, 83–273 K, have been measured by Korf.<sup>12</sup> The value of  $S^\circ(298.15 \text{ K})$  is derived based on the adopted low temperature heat capacities, using  $S^\circ(2.86 \text{ K}) = 0.0033 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ .

The high temperature enthalpies were determined by Skuratov and Lapushkin,<sup>13</sup> 623–923 K, Dworkin,<sup>14</sup> 854–954 K; and Cooper,<sup>15</sup> 297–973 K. Heat capacities are derived from the enthalpies by a curve fitting method which requires a smooth joint with the low temperature  $C_p$ . Enthalpy values used in the curve fit include smooth values calculated from the equation of Skuratov and the value  $H_f^\circ(954) - H_f^\circ(298.15) = 9.2 \text{ kcal}\cdot\text{mol}^{-1}$  from Dworkin. Deviation of the input values from the selected enthalpies are all less than 0.3 percent, while the deviations of the data of Cooper range from +1.0 at 570 K to -1.6 percent at 974 K. Since the latter point is 20 above the melting point, there appears to be an error in Cooper's measurement of temperature.  $C_p$  above the melting point is obtained by graphical extrapolation.

## Fusion Data

$T_{\text{fus}}$  has been reported to be 953, 952, and 954 K by Ray and Dayal,<sup>16</sup> Phipps and Partridge,<sup>17</sup> and Johnson and Bredig,<sup>18</sup> respectively. The latter value is adopted. The enthalpy of fusion was determined by Dworkin and Bredig,<sup>19</sup> using drop calorimetry.

## Sublimation Data

The difference between  $\Delta_fH^\circ(298.15 \text{ K})$  for KI(g) and KI(cr) is  $\Delta_{\text{sub}}H^\circ$  (to monomer, 298.15 K). The  $\Delta_{\text{sub}}H^\circ$  (to dimer, 298.15 K K) is calculated as the enthalpy change for the following reaction:  $2\text{KI}(\text{cr}) = \text{K}_2\text{I}_2(\text{g})$ .

## References

- V. B. Parker, NSRDS NBS 2, 66 pp. (1965).
- U. S. Nat. Bur. Stand. Tech. Note 124 pp., (1965).
- J. Thomsen, Thermochemische Untersuchungen, J. Barth Verlag, Leipzig, 1882–86.
- J. Wust and E. Lange, Z. Physik. Chem. 116, 161 (1925).
- E. Lange and W. Martin, Z. Physik. Chem. A180, 233 (1937).
- M. M. Popov, S. M. Skuratov, and M. M. Sirel'tsova, Zhur. Obshch. Khim. 10, 2023 (1940).
- M. Bobelsky and R. D. Lairsch, J. Chem. Soc. 1950, 3612 (1950).
- A. F. Kapustinskii and S. I. Drakin, Zhur. Fiz. Khim. 26, 581 (1952).
- W. T. Berg and J. A. Morrison, Proc. Roy. Soc. (London) A242, 467 (1957).
- W. S. Scales, Phys. Rev. 112, 49 (1958).
- K. Clausius, J. Goldmann, and A. Perlick, Z. Naturforsch. 4A, 424 (1949).
- S. M. Skuratov and S. A. Lapushkin, Russ. J. Gen. Chem. 21, 2485 (1951).
- A. S. Dworkin, Oak Ridge National Laboratory, personal communication, (December 1, 1964).
- C. B. Cooper, J. Chem. Phys. 21, 777 (1953).
- R. C. Ray and V. Dayal, Trans. Faraday Soc. 32, 741 (1936).
- T. E. Phipps and E. G. Partridge, J. Amer. Chem. Soc. 51, 1331 (1929).
- J. W. Johnson and M. A. Bredig, J. Phys. Chem. 62, 604 (1958).
- A. S. Dworkin and M. A. Bredig, J. Phys. Chem. 64, 269 (1960).

T/K	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>1</sub>
	C <sub>p</sub> <sup>a</sup>	S° - [G° - H°(T)]/T	H° - H°(T)	Δ <sub>f</sub> H°	
0	0	0	INFINITE	-326.930	INFINITE
100	43.003	52.413	151.616	-327.397	170.300
200	50.518	85.772	111.148	-327.612	84.770
298.15	52.777	106.387	106.387	-327.900	56.592
300	52.806	106.713	106.388	-327.907	56.238
400	53.932	122.054	108.472	-338.870	41.859
500	55.363	134.235	112.446	-360.614	32.790
600	57.300	144.490	116.953	-359.903	304.584
700	59.777	153.503	121.543	-358.933	298.437
800	62.639	161.668	126.055	-357.681	18.703
900	65.793	169.225	130.437	-356.140	-277.653
954.000	67.594	173.111	132.743	38.510	---
1000	69.036	176.329	134.674	41.654	---
1100	71.546	183.033	138.769	48.691	14.051
1200	73.136	189.332	142.723	53.930	12.155
1300	74.090	195.226	146.537	57.285	10.455
1400	74.601	200.737	150.214	70.733	9.077
1500	74.927	205.895	153.756	78.209	7.813
1600	75.145	210.739	157.168	85.713	6.770
1700	75.254	215.297	160.454	93.232	5.864
1800	75.291	219.599	163.622	100.759	5.072
1900	75.317	223.671	166.676	108.290	4.373
2000	75.312	227.534	169.623	115.821	3.750

PREVIOUS December 1961

CURRENT June 1967

## Potassium Iodide (KI)

I<sub>1</sub>K<sub>1</sub>(cr)

Potassium Iodide (KI)

LIQUID

$M_r = 166.0028$  Potassium Iodide (KI)

$I_1K_1(l)$

$S^\circ(298.15\text{ K}) = [114.098] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = 954\text{ K}$

$\Delta H_f^\circ(298.15\text{ K}) = [-312.846] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{vap}}H^\circ = 24.016 \text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation

$\Delta_f H^\circ(\text{KI}, l, 298.15\text{ K})$ , is calculated from  $\Delta_f H^\circ(\text{KI}, \text{cr}, 298.15\text{ K})$  by adding the enthalpy of fusion,  $\Delta_{\text{fus}}H^\circ$ , and the difference in enthalpy,  $H^\circ(954\text{ K}) - H^\circ(298.15\text{ K})$ , between the crystal and liquid.

Heat Capacity and Entropy

The heat capacity is derived as  $17.3 \text{ cal K}^{-1}\cdot\text{mol}^{-1}$  from the enthalpy measurements, 954-1014K, by Dworkin.<sup>1</sup> This  $C_p^\circ$  value is adopted in the temperature range 298.15 K.  $S^\circ(298.15\text{ K})$  is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion Data

Refer to the crystal table for details.

Vaporization Data

The boiling point,  $T_{\text{vap}} = 1618\text{ K}$  (1 atm), is calculated as the temperature at which the sum of the partial pressure of KI(g) and  $K_2I_2(g)$  over KI(l) equals one atmosphere. The value of  $\Delta_{\text{vap}}H^\circ$  is calculated as the heat required to produce one mole of vapor mixture, which contains 78 percent monomer (KI) and 22 percent dimer ( $K_2I_2$ ) at  $T_{\text{vap}}$ .

$T_{\text{vap}}$  was reported as 1603 and 1590 K by Wartenberg and Albrecht,<sup>2</sup> and Ruff and Muggdan,<sup>3</sup> respectively.

References

- <sup>1</sup>A.S. Dworkin, Oak Ridge National Laboratory, personal communication, (December 1, 1964).
- <sup>2</sup>H von Wartenberg and P. Albrecht, Z. Elektrochem. 27, 162 (1921).
- <sup>3</sup>O. Ruff and S. Jügdan, Z. Anorg Chem 117, 147 (1921).

T/K	$C_p^\circ$	$S^\circ$	$S^\circ - [G^\circ - H^\circ(T)]/T$	$H^\circ - H^\circ(T)$	$\Delta_f H^\circ$	$\Delta G^\circ$	$\log K_f$
0				0.			
100				0.134	-312.846	-310.269	54.358
200				0.372	-312.817	-310.253	54.020
298.15	72.383	114.098	114.100	0.7372	-321.876	-308.881	40.336
300	72.383	114.546	116.939	1.4611	-341.844	-303.743	31.732
400	72.383	135.369	122.300	21.849	-339.522	-296.340	25.799
500	72.383	151.521	128.303	29.087	-337.163	-289.329	21.590
600	72.383	164.718	134.325	34.326	-334.792	-282.637	18.456
700	72.383	175.876	140.155	43.564	-332.431	-276.282	16.035
800	72.383	183.541	145.663	47.473	---	---	---
900	72.383	194.067	148.523	50.802	---	---	---
954.000	72.383	198.285	150.891	58.040	-330.106	-270.169	14.112
1000	72.383	201.693	155.828	65.279	-406.794	-259.675	12.331
1100	72.383	208.592	160.491	72.517	-403.551	-246.444	10.727
1200	72.383	214.890	164.902	79.755	-400.320	-233.483	9.381
1300	72.383	220.684	169.090	86.994	-397.104	-220.770	8.237
1400	72.383	226.048	173.046	94.232	-393.909	-208.286	7.253
1500	72.383	231.042	176.819	101.470	-390.740	-196.015	6.399
1600	72.383	235.714	180.413	108.709	-387.602	-183.941	5.652
1700	72.383	240.102	183.845	115.947	-384.499	-172.051	4.993
1800	72.383	244.239	187.128	123.185	-381.435	-160.332	4.408
1900	72.383	248.153	190.273	130.424	-378.411	-148.773	3.886
2000	72.383	251.866	193.291	137.365	-375.428	-137.365	3.417
2100	72.383	255.397	196.191	144.982	-372.488	-126.098	2.994
2200	72.383	258.764	198.982	152.159	-369.581	-114.983	2.511
2300	72.383	261.982	201.671	159.377	-366.715	-103.925	2.053
2400	72.383	265.063	204.267	193.577	-363.879	-93.065	1.544
2500	72.383	268.017	204.267				

PREVIOUS: December 1961

CURRENT: June 1967

Potassium Iodide (KI)

$I_1K_1(l)$

Potassium Iodide (KI)

CRYSTAL-LIQUID

0 to 954 K crystal  
above 954 K liquid

Refer to the individual tables for details.

$M_r = 166.0028$  Potassium Iodide (KI)

$I_r(K_1(cr,l))$

T/K	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa		$\log K_r$
	$C_p^\circ$	$S^\circ - (G^\circ - H^\circ(T_r))/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	
J·K <sup>-1</sup> ·mol <sup>-1</sup>					
0	0	INFINITE	-12.711	-326.930	INFINITE
100	45.003	52.413	-9.970	-327.397	170.300
200	50.518	85.772	-5.075	-327.612	84.770
298.15	52.777	106.387	0	-327.900	56.592
300	52.806	106.713	0.098	-327.907	56.238
400	53.932	122.054	5.433	-338.870	41.859
500	55.363	134.235	10.894	-360.614	32.790
600	57.300	144.490	16.572	-359.903	26.516
700	59.777	153.503	22.372	-358.933	22.046
800	62.639	161.668	28.490	-357.681	18.703
900	65.793	169.225	34.909	-356.140	16.113
954.000	67.594	173.111	38.510	CRYSTAL $\leftarrow$ LIQUID	---
954.000	72.383	198.285	62.527	TRANSITION	---
1000	72.383	201.693	65.856	-330.106	14.112
1100	72.383	208.592	73.095	-406.794	-259.675
1200	72.383	214.890	80.333	-403.531	-246.444
1300	72.383	220.684	87.571	-400.320	-233.483
1400	72.383	226.048	94.810	-397.104	-220.770
1500	72.383	231.042	102.048	-393.909	-208.286
1600	72.383	235.714	109.286	-390.740	-196.015
1700	72.383	240.102	116.524	-387.602	-183.941
1800	72.383	244.239	123.763	-384.499	-172.051
1900	72.383	248.153	131.001	-381.435	-160.332
2000	72.383	251.866	138.239	-378.411	-148.773
2100	72.383	255.397	145.478	-375.428	-137.365
2200	72.383	258.764	152.716	-372.485	-126.098
2300	72.383	261.982	159.954	-369.581	-114.963
2400	72.383	265.063	167.193	-366.713	-103.955
2500	72.383	268.017	174.431	-363.879	-93.065

PREVIOUS:

CURRENT June 1967

Potassium Iodide (KI)

$I_r(K_1(cr,l))$

Potassium Iodide (KI)

$M_r = 166.0028$  Potassium Iodide (KI)

$I_1(K)(g)$

$S^\circ(298.15\text{ K}) = 258.283\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   $\Delta_f H^\circ(0\text{ K}) = -122.08 \pm 2.1\text{ kJ}\cdot\text{mol}^{-1}$   $\Delta_f H^\circ(298.15\text{ K}) = -125.52 \pm 2.1\text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum Weight	
State	$\epsilon_n, \text{cm}^{-1}$
$\Sigma^+$	0

$\omega_e x_e = 186.287 \pm 0.04\text{ cm}^{-1}$   $\sigma = 1$   
 $B_e = 0.06072\text{ cm}^{-1}$   $\alpha_e = 0.000267\text{ cm}^{-1}$   $r_e = 3.0478\text{ \AA}$

Enthalpy of Formation

The enthalpy of formation is derived from the sublimation and vaporization data analyzed below. Many investigators have determined the total pressures of KI(g) and  $K_2I_2(g)$  over KI(cr) or KI(l) by static methods or "apparent" pressures by Knudsen effusion or transpiration. These pressures are converted to monomer pressures by use of functions [refer to  $K_2I_2(g)$  table] which are consistent with the dimer monomer equilibrium data of Datz.<sup>9</sup> 2nd and 3rd law analyses of the monomer pressures show reasonable agreement. The selected value of  $\Delta_f H^\circ(298.15\text{ K}) = -30.0 \pm 0.5\text{ kcal}\cdot\text{mol}^{-1}$  is also in good agreement with  $-30.23 \pm 1.15$  and  $-30.46\text{ kcal}\cdot\text{mol}^{-1}$  derived from  $D_0^\circ = 3.32 \pm 0.05$  and  $3.33\text{ eV}$  reported by Gaydon<sup>10</sup> and Herzberg<sup>11</sup>, respectively.

Source	Reactions*	T/K	Data Points	$\Delta_f H^\circ(298.15\text{ K}), \text{kcal}\cdot\text{mol}^{-1}$	Drift $\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\Delta_f H^\circ(298.15\text{ K}), \text{kcal}\cdot\text{mol}^{-1}$
Wartenberg-Albrecht <sup>1</sup>	(B)	1336.2-1606.2	9	$47.79 \pm 0.38$	$-2.1 \pm 0.2$	-30.01
Ruff-Mugdan <sup>2</sup>	(B)	1319.2-1590.2	12	$49.38 \pm 1.03$	$-3.3 \pm 0.7$	-30.18
Flock-Rodebush <sup>3</sup>	(B)	1116.1-1275.7	8	$45.43 \pm 0.03$	$-0.6 \pm 0.1$	-30.02
Greiner-Jellinek <sup>4</sup>	(B)	1453.2	1	-	-	-29.53
Niwa <sup>5</sup>	(A)	803.2-873.2	8	$46.11 \pm 0.35$	$2.6 \pm 0.4$	-30.07
Zimm-Mayer <sup>6</sup>	(A)	618.4-892.9	10	$48.66 \pm 0.25$	$-0.4 \pm 0.3$	-29.90
Cogin-Kimball <sup>7</sup>	(A)	721.5-897.7	29	$48.52 \pm 0.40$	$1.1 \pm 0.5$	-30.64
Bridgers <sup>8</sup>	(A)	697.5-891.7	25	$48.48 \pm 0.22$	$-1.1 \pm 0.3$	-30.65

\*Reactions: (A) KI(cr) = KI(g); (B) KI(l) = KI(g).

Heat Capacity and Entropy

The ground state configuration is obtained from Herzberg.<sup>11</sup> The adopted values of  $\omega_e, \omega_e x_e, B_e, \alpha_e,$  and  $r_e$  were determined using millimeter wave molecular beam spectroscopy by Rusk and Gordy<sup>12</sup> and corrected to the average isotopic species. Similar values were reported by Honig *et al.*<sup>13</sup> from microwave spectra, except  $\omega_e$ , which was given as  $199.74\text{ cm}^{-1}$ . The value of  $\omega_e$  was derived to be  $200$  and  $173\text{ cm}^{-1}$  by Barrow and Caunt<sup>14</sup> and Rice and Klemperer.<sup>15</sup> The moment of inertia is  $4.5979 \times 10^{-38}\text{ g cm}^2$ .

References

- H. von Wartenberg and P. Albrecht, *Z. Elektrochem.* **27**, 162 (1921).
- O. Ruff and S. Mugdan, *Z. Anorg. Chem.* **117**, 147 (1921).
- E. F. Flock and W. H. Rodebush, *J. Amer. Chem. Soc.* **48**, 2522 (1926).
- B. Greiner and K. Jellinek, *Z. Physik. Chem. (Leipzig)* **A165**, 97 (1933).
- K. Niwa, *J. Fac. Sci. Hokkaido Imperial Univ., Ser. III*, **2**, 201 (1938).
- B. H. Zimm and J. E. Mayer, *J. Chem. Phys.* **12**, 362 (1944).
- G. E. Cogin and G. E. Kimball, *J. Chem. Phys.* **16**, 1035 (1948).
- H. E. Bridgers, Ph.D. Thesis, The Ohio State University, (1953).
- S. Datz, Oak Ridge National Laboratory, ORNL 2933, (1960).
- A. G. Gaydon, "Dissociation Energies and Spectra of Diatomic Molecules," 2nd ed., Chapman and Hall Ltd., London, 261 pp. (1953).
- G. Herzberg, "Spectra of Diatomic Molecules," D. Van Nostrand Co., Inc., New York, (1950).
- J. R. Rusk and W. Gordy, *Phys. Rev.* **127**, 817 (1962).
- A. Honig, M. Mandel, M. L. Stich and C. H. Townes, *Phys. Rev.* **96**, 629 (1954).
- R. F. Barrow and A. D. Caunt, *Proc. Roy. Soc. (London)* **A219**, 120 (1953).
- S. A. Rice and W. Klemperer, *J. Chem. Phys.* **27**, 573 (1957).

T/K	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$		log K <sub>r</sub>
	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f G^\circ$	
0	0	INFINITE	INFINITE	-122.081	INFINITE
100	33.908	219.083	290.729	-71.854	39.775
200	36.441	243.584	261.662	-123.772	33.290
250	36.869	251.766	258.893	-1.782	29.071
298.15	37.122	258.283	258.283	0	28.935
300	37.130	258.513	258.182	-125.556	28.935
350	37.308	262.251	258.737	-128.992	25.785
400	37.439	269.241	259.745	-138.124	23.333
450	37.543	273.657	261.050	-139.830	18.644
500	37.629	277.617	265.512	-161.576	19.486
600	37.771	284.491	265.619	-162.722	16.663
700	37.889	290.322	268.742	-163.818	14.633
800	37.994	295.389	271.763	-164.891	13.100
900	38.093	299.870	274.692	-165.964	11.900
1000	38.186	303.888	277.569	-167.064	10.934
1100	38.277	307.532	279.948	-247.167	9.919
1200	38.366	310.866	282.388	-247.330	8.941
1300	38.453	313.940	284.698	-247.496	8.112
1400	38.539	316.793	286.890	-247.669	7.402
1500	38.624	319.455	288.973	-247.854	6.785
1600	38.709	321.951	290.957	-248.056	6.246
1700	38.793	324.300	292.850	-248.282	5.769
1800	38.877	326.520	294.660	-248.534	5.345
1900	38.961	328.624	296.392	-248.816	4.965
2000	39.044	330.624	298.054	-249.130	4.623
2100	39.128	332.531	299.651	-249.477	4.313
2200	39.211	334.353	301.187	-249.856	4.031
2300	39.294	336.098	302.667	-250.265	3.773
2400	39.377	337.772	304.095	-250.702	3.536
2500	39.459	339.381	305.475	-251.163	3.317
2600	39.542	340.931	306.809	-251.647	3.115
2700	39.625	342.425	308.101	-252.149	2.928
2800	39.707	343.867	309.352	-252.668	2.753
2900	39.790	345.262	310.561	-253.201	2.591
3000	39.872	346.612	311.746	-253.746	2.438
3100	39.955	347.921	312.892	-254.300	2.296
3200	40.037	349.191	314.006	-254.872	2.162
3300	40.119	350.424	315.091	-255.445	2.035
3400	40.202	351.623	316.148	-256.037	1.916
3500	40.284	352.790	317.179	-256.642	1.804
3600	40.366	353.925	318.184	-257.266	1.697
3700	40.449	355.033	319.165	-257.912	1.596
3800	40.531	356.112	320.123	-258.583	1.500
3900	40.613	357.166	321.059	-259.283	1.409
4000	40.696	358.196	321.975	-260.011	1.322
4100	40.778	359.201	322.871	-260.778	1.239
4200	40.860	360.185	323.747	-261.593	1.160
4300	40.942	361.148	324.606	-262.457	1.084
4400	41.025	362.090	325.447	-263.369	1.012
4500	41.107	363.013	326.272	-264.306	0.942
4600	41.189	363.917	327.080	-265.268	0.876
4700	41.271	364.804	327.874	-266.256	0.812
4800	41.353	365.673	328.652	-267.269	0.750
4900	41.436	366.527	329.416	-268.301	0.691
5000	41.518	367.365	330.167	-269.359	0.633
5100	41.600	368.188	330.904	-270.426	0.578
5200	41.682	368.996	331.629	-271.528	0.525
5300	41.764	369.791	332.342	-272.661	0.473
5400	41.846	370.573	333.044	-273.823	0.423
5500	41.929	371.341	333.732	-275.022	0.375
5600	42.011	372.097	334.410	-276.252	0.328
5700	42.093	372.842	335.078	-277.519	0.283
5800	42.175	373.574	335.735	-278.820	0.238
5900	42.257	374.296	336.383	-280.156	0.196
6000	42.339	375.007	337.021	-281.524	0.154

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

Potassium Iodide (KI)

$I_1(K)(g)$

## Lithium iodide (Lil)

## CRYSTAL

 $M_r = 133.8455$ 

## Lithium Iodide (Lil)

 $i, Li_1(cr)$ 

$S^\circ(298.15\text{ K}) = [85.772] \text{ J K}^{-1} \cdot \text{mol}^{-1}$   
 $T_{\text{fus}} = 742 \text{ K}$   
 $\Delta H_f^\circ(0 \text{ K}) = \text{Unknown}$   
 $\Delta H_f^\circ(298.15 \text{ K}) = -270.08 \pm 0.4 \text{ kJ} \cdot \text{mol}^{-1}$   
 $\Delta_{\text{ion}} H^\circ = 14.644 \text{ kJ} \cdot \text{mol}^{-1}$

## Enthalpy of Formation

The enthalpy of formation,  $\Delta_f H^\circ(\text{Lil}, cr, 298.15 \text{ K}) = -64.55 \text{ kcal} \cdot \text{mol}^{-1}$ , was calculated from the heat of solution of lithium iodide (cr) at infinite dilution and the ionic heats of formation of  $\text{Li}^+(\text{aq}, \infty)$  and  $\text{I}^-(\text{aq}, \infty)$ .

Parker<sup>1</sup> reviewed the literature heat of solution data and gave the "best" value,  $\Delta_{\text{ion}} H^\circ(\text{aq}, \text{limf}) = -15.130 \pm 75 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  for  $\text{LiI}(cr) \rightarrow \text{Li}^+(\text{aq}, \text{limf})$  at 298.15 K. The ionic heat of formation,  $\Delta_f H^\circ(\text{Li}^+, \text{aq}, \infty, 298.15 \text{ K}) = -66.49 \text{ kcal} \cdot \text{mol}^{-1}$  was calculated from  $\Delta_f H^\circ(\text{LiOH}, \text{aq}, \infty, 298.15 \text{ K}) = -121.46 \text{ kcal} \cdot \text{mol}^{-1}$  (see JANAF-LiOH(cr) table, Mar 31, 1966) with  $\Delta_f H^\circ(\text{OH}^-, \text{aq}, \infty, 298.15 \text{ K}) = -54.97 \text{ kcal} \cdot \text{mol}^{-1}$  from<sup>2</sup>. The value  $\Delta_f H^\circ(\text{I}^-, \text{aq}, \infty, 298.15 \text{ K}) = 13.19 \text{ kcal} \cdot \text{mol}^{-1}$  was also obtained from<sup>3</sup>. Combination of the ionic heats of formation of  $\text{Li}^+(\text{aq}, \infty)$  and  $\text{I}^-(\text{aq}, \infty)$  gives the heat of formation of  $\text{LiI}(\text{aq}, \infty)$ ,  $\Delta_f H^\circ(298.15 \text{ K}) = -79.68 \text{ kcal} \cdot \text{mol}^{-1}$ .

## Heat Capacity and Entropy

Dworkin<sup>4</sup> has measured the enthalpy changes by the drop method (642–802 K), yielding  $H^\circ(742 \text{ K}) - H^\circ(298.15 \text{ K}) = 6.0 \text{ kcal} \cdot \text{mol}^{-1}$  for the crystal at the melting point. Heat capacities derived from his data were  $C_p^\circ(692 \text{ K}) = 14.8$  and  $C_p^\circ(772 \text{ K}) = 15.1 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  for the crystal and liquid, respectively. The tabulated heat capacities were estimated based on these values and on the heat capacities of  $\text{LiCl}(cr)$ ,  $\text{NaCl}(cr)$  and  $\text{NaI}(cr)$ .

The entropy,  $S^\circ(298.15 \text{ K}) = 20.5 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ , was estimated by adding the entropy difference at 298.15 K between  $\text{NaI}(cr)$  and  $\text{NaCl}(cr)$  to the entropy of  $\text{LiCl}(cr)$ . Comparisons with other alkali halides give results within  $\pm 0.5 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$  of this value.

Kelley<sup>5</sup> has estimated the heat capacities ( $C_p^\circ = 12.30 + 2.44 \times 10^{-3} T \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ ) and the entropy,  $S^\circ(298.15 \text{ K}) = 17.50 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ .

## Fusion Data

The selected enthalpy of fusion,  $\Delta H_f^\circ(823 \text{ K}) = 350 \text{ kcal} \cdot \text{mol}^{-1}$  was obtained from enthalpy measurements in a drop calorimeter by Dworkin and Bredig.<sup>6</sup>

## References

- <sup>1</sup>V. B. Parker, NSRDS NBS 2, 66 pp. (1965).
- <sup>2</sup>J. S. Nat. Bur. Stand. Tech. Note 270-1, 124 pp. (1965).
- <sup>3</sup>A. S. Dworkin, Oak Ridge National Laboratory, personal communication, (December, 1964).
- <sup>4</sup>K. K. Kelley, U. S. Bur. Mines Bull. 584, 1960; U.S. Bur. Mines Bull. 592, 149 pp. (1961).
- <sup>5</sup>A. S. Dworkin and M. A. Bredig, J. Phys. Chem. 64, 269 (1960).

T/K	$C_p^\circ$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$		$\log K_f$
		$S^\circ - [G^\circ - F^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0			0.			
100	50.082	85.772	0.093	-270.077	-269.665	47.244
200	50.187	86.082	5.243	-270.080	-269.662	46.952
300	53.430	100.875	10.714	-278.350	-269.208	35.155
400	55.948	113.073	16.437	-302.910	-264.545	27.637
500	58.660	123.099	22.480	-309.047	-256.948	22.369
600	62.658	131.807	28.891	-300.814	-249.573	18.620
700	66.107	141.363	35.680	-299.188	-242.302	15.821
800	69.517	149.355	42.763	-297.185	-235.308	13.651
900	71.965	156.815	50.042	-292.399	-228.553	11.938
1000	73.534	163.751	57.448	-289.785	-222.039	10.544
1100	74.559	170.195	64.946	-287.087	-215.757	9.392
1200	75.375	176.196	72.510	-284.333	-209.697	8.426
1300	75.877	181.801	80.116	-281.548	-203.847	7.606
1400	76.191	187.049	87.735	-278.767	-198.195	6.902
1500	76.191	191.966	95.354	-275.999	-192.729	6.292
1600	76.191	196.585	102.974	-273.243	-187.461	5.739
1700	76.191	200.940	110.593	-270.500	-182.261	5.239
1800	76.191	205.060	118.212	-267.766	-177.102	4.823
1900	76.191	208.968	125.831	-265.009	-172.072	4.487
2000	76.191	212.685	133.450	-262.229	-167.165	4.211
2100	76.191	216.229	141.069	-259.424	-162.354	3.982
2200	76.191	219.616	148.688	-256.591	-157.626	3.792
2300	76.191	222.859	156.307	-253.729	-153.000	3.632
2400	76.191	225.969	163.946	-250.847	-148.482	3.500
2500	76.191	228.969	171.600	-247.947	-144.066	3.392
						3.314

PREVIOUS: September 1961

CURRENT: June 1966

## Lithium Iodide (Lil)

 $i, Li_1(cr)$



LIQUID

***M<sub>r</sub>* = 133.8455 Lithium Iodide (LiI)**

***I<sub>1</sub>*Li<sub>1</sub>(l)**

*S*<sup>o</sup>(298.15 K) = [98.611] J·K<sup>-1</sup>·mol<sup>-1</sup>      Δ<sub>liq</sub>*H*<sup>o</sup>(298.15 K) = [-258.349] kJ·mol<sup>-1</sup>  
*T<sub>liq</sub>* = 742 K      Δ<sub>liq</sub>*H*<sup>o</sup> = 14.644 kJ·mol<sup>-1</sup>

**Enthalpy of Formation**

Δ<sub>liq</sub>*H*<sup>o</sup>(LiI, l, 298.15 K) is calculated from Δ<sub>liq</sub>*H*<sup>o</sup>(LiI, cr, 298.15 K) by adding the enthalpy of fusion, Δ<sub>fus</sub>*H*<sup>o</sup>, and the difference in enthalpy, *H*<sup>o</sup>(742 K) - *H*<sup>o</sup>(298.15 K), between the crystal and liquid.

**Heat Capacity and Entropy**

Dworkin<sup>1</sup> has derived the heat capacity (*C<sub>p</sub>*<sup>o</sup> = 15.1 cal·K<sup>-1</sup>·mol<sup>-1</sup>) from enthalpy measurements (742–802 K) by the drop method. The liquid heat capacity was assumed to be constant as 15.1 cal·K<sup>-1</sup>·mol<sup>-1</sup>. The entropy at 298.15 K is calculated in a manner analogous to that used for the enthalpy of formation.

**Fusion Data**

Refer to the crystal table for details.

**Vaporization Data**

*T<sub>sat</sub>*(to monomer only) = 1497 K is determined as the temperature at which the fugacity is 1 atm for the reaction LiI(l) = LiI(g). The corresponding enthalpy change (Δ<sub>vap</sub>*H*<sup>o</sup>) at boiling point is the enthalpy of vaporization Δ<sub>vap</sub>*H*<sup>o</sup>(to monomer only).

*T<sub>sat</sub>*(to equilibrium mixture) = 1447 K is the temperature at which the sum of the calculated partial vapor pressures of LiI(g) and Li<sub>2</sub>I<sub>2</sub>(g) reaches one atmosphere (trimer and higher polymer have been neglected in calculation). This value is in good agreement with the boiling point of 1444 K from the least squares fit of the total vapor pressure data measured by Ruff and Muggdan.<sup>2</sup> Δ<sub>vap</sub>*H*<sup>o</sup>(to equilibrium mixture) at the boiling point is calculated as the heat of vaporization of one mole of liquid to vapor containing 30.44 mole percent of dimer. For detailed information see LiI(g) and Li<sub>2</sub>I<sub>2</sub>(g) tables.

**References**

- <sup>1</sup>A. S. Dworkin, Oak Ridge National Laboratory, personal communication, (December 1964).
- <sup>2</sup>O. Ruff and S. Muggdan, Z. Anorg. Chem. 117, 147 (1921).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa	
	<i>C<sub>p</sub></i> <sup>o</sup>	<i>S</i> <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	log <i>K<sub>f</sub></i>
0				
100				
200				
298.15	63.178	98.611	0.	-261.764
300	63.178	98.612	0.117	-258.349
400	63.178	117.177	6.435	-261.785
500	63.178	131.275	12.753	-265.430
600	63.178	142.794	19.070	-268.809
700	63.178	152.533	25.388	-269.143
742.000	63.178	156.214	28.042	-254.163
800	63.178	160.969	31.706	-248.694
900	63.178	168.410	38.024	---
1000	63.178	175.067	44.342	CRYSTAL <--- LIQUID
1100	63.178	181.088	50.660	-284.644
1200	63.178	186.586	56.977	-283.113
1300	63.178	191.643	63.295	-238.386
1400	63.178	196.325	69.613	-233.498
1500	63.178	200.683	75.931	-228.764
1600	63.178	204.761	82.249	-224.104
1700	63.178	208.593	88.567	-220.600
1800	63.178	212.202	94.884	-217.200
1900	63.178	215.618	101.202	-213.886
2000	63.178	218.859	107.520	-210.650
2100	63.178	221.941	113.838	-207.485
2200	63.178	224.880	120.156	-204.389
2300	63.178	227.689	126.474	-201.351
2400	63.178	230.378	132.792	-198.372
2500	63.178	232.957	139.109	-195.454

PREVIOUS: September 1961

CURRENT: June 1966

Lithium Iodide (LiI)

***I<sub>1</sub>*Li<sub>1</sub>(l)**

CRYSTAL-LIQUID

Lithium Iodide (LiI)

0 to 742 K crystal  
above 742 K liquid

Refer to the individual tables for details.

$M_r = 133.8455$  Lithium Iodide (LiI)

$I_1Li_1(cr,l)$

T/K	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^* = 0.1$ MPa		$\log K_f$
		$S^* - [C_p^* - H^*(T_r)]/T$	$H^* - H^*(T_r)$	$\Delta H_f^*$	$\Delta G_f^*$	
		J·K <sup>-1</sup> ·mol <sup>-1</sup>		kJ·mol <sup>-1</sup>		
0						
100						
200						
298.15	50.082	85.772	85.772	0.	-270.077	-269.665
300	50.187	86.082	85.773	0.093	-270.080	-269.662
400	53.430	100.875	87.767	5.243	-278.350	-269.208
500	55.948	113.073	91.645	10.714	-302.910	-264.545
600	58.660	123.499	96.104	16.437	-302.047	-256.948
700	62.258	132.807	100.693	22.480	-300.814	-249.523
742.000	63.764	136.478	102.615	25.126	CRYSTAL $\leftarrow$ LIQUID	18.620
742.000	63.178	136.214	102.615	39.770	TRANSITION	
800	63.178	160.969	106.676	43.435	-284.644	15.895
900	63.178	168.410	113.130	49.752	-283.113	13.836
1000	63.178	175.067	118.997	56.070	-281.582	12.197
1100	63.178	181.088	124.372	62.388	-280.053	10.863
1200	63.178	186.586	129.331	68.706	-278.527	9.758
1300	63.178	191.643	133.932	75.024	-277.010	8.828
1400	63.178	196.325	138.224	81.342	-275.502	8.035
1500	63.178	200.684	142.244	87.659	-274.005	7.351
1600	63.178	204.761	146.025	93.977	-272.525	6.757
1700	63.178	208.591	149.594	100.295	-271.062	6.014
1800	63.178	212.202	152.973	106.613	-269.616	5.305
1900	63.178	215.618	156.181	112.931	-268.188	4.674
2000	63.178	218.859	159.234	119.249	-266.781	4.110
2100	63.178	221.941	162.148	125.566	-265.395	3.601
2200	63.178	224.880	164.933	131.884	-264.031	3.141
2300	63.178	227.689	167.601	138.202	-262.688	2.723
2400	63.178	230.378	170.161	144.520	-261.366	2.342
2500	63.178	232.957	172.622	150.838	-260.065	1.993

PREVIOUS:

CURRENT: June 1966

Lithium Iodide (LiI)

$I_1Li_1(cr,l)$

IDEAL GAS

Lithium Iodide (LiI)

$M_r = 133.8455$  Lithium Iodide (LiI)

$I_2Li_2(g)$

$S^\circ(298.15\text{ K}) = 232.262\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   $\Delta_f H^\circ(0\text{ K}) = -89.08 \pm 8.4\text{ kJ}\cdot\text{mol}^{-1}$   $\Delta_f H^\circ(298.15\text{ K}) = -91.00 \pm 8.4\text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum State	Weight $g_i$
$1\Sigma^+$	1

$\omega_e = 498.16\text{ cm}^{-1}$   $\omega_e x_e = 3.39\text{ cm}^{-1}$   $\sigma = 1$   
 $B_e = 0.44837\text{ cm}^{-1}$   $\alpha_e = 0.00416\text{ cm}^{-1}$   $r_e = 2.3919\text{ \AA}$

Enthalpy of Formation

The enthalpy of formation,  $\Delta_f H^\circ(\text{LiI}_2, g, 298.15\text{ K}) = -21.75 \pm 2\text{ kcal}\cdot\text{mol}^{-1}$ , was calculated from the selected heat of sublimation and the enthalpy of formation for lithium iodide (cr). The heat of sublimation has been determined mass spectrometrically from the ion intensity measurement (2nd law method) by Gorokhov as  $\Delta_{\text{sub}} H^\circ(\text{cr} \rightarrow \text{monomer}, 298.15\text{ K}) = 42.9 \pm 0.6$  and  $\Delta_{\text{sub}} H^\circ(\text{cr} \rightarrow \text{dimer}, 298.15\text{ K}) = 43.2 \pm 0.4\text{ kcal}\cdot\text{mol}^{-1}$  in the temperature range from 626–722 K. Gorokhov also reported the partial vapor pressure of monomeric lithium iodide ( $P_{\text{monomer}} = 3 \times 10^{-3}\text{ mm Hg}$ ) and the ratio of dimer to monomer ( $P_{\text{dimer}}/P_{\text{monomer}} = 6$ ) which have been used for 3rd law calculation. Using the same technique, Friedman reported the heats of sublimation as  $\Delta_{\text{sub}} H^\circ(\text{cr} \rightarrow \text{monomer}, 727\text{ K}) = 41.9 \pm 0.5$  and  $\Delta_{\text{sub}} H^\circ(\text{cr} \rightarrow \text{dimer}, 727\text{ K}) = 40.8 \pm 0.5\text{ kcal}\cdot\text{mol}^{-1}$  in the temperature range from 630 to 730 K. Berkowitz *et al.* have also studied the lithium iodide vapor in the mass spectrometer and reported the 2nd law and 3rd law values of the heat of dimerization at 800 K as 37.9 and 40.4 kcal·mol<sup>-1</sup>, respectively. Using the JANAF thermodynamic functions, all the heats of sublimation and dimerization at different temperatures have been reduced to 298.15 K and summarized in the following table. The total vapor pressure over the liquid has been measured by a boiling point method in the temperature range 1223 to 1413 K by Ruff and Mugdan<sup>6</sup> (Their data have been quoted by Wartenberg and Schulz.<sup>7</sup>) In order to have good agreement between the calculated vapor pressure and the observed total vapor pressure, the heats of sublimation have been chosen as  $\Delta_{\text{sub}} H^\circ(298.15\text{ K}) = 42.8\text{ kcal}\cdot\text{mol}^{-1}$  and  $\Delta_{\text{sub}} H^\circ(\text{cr} \rightarrow \text{dimer}, 298.15\text{ K}) = 42.6\text{ kcal}\cdot\text{mol}^{-1}$  and the heat of dissociation of dimer,  $\Delta_d H^\circ(\text{cr} \rightarrow \text{monomer}, 298.15\text{ K}) = 43.0\text{ kcal}\cdot\text{mol}^{-1}$ . The calculated boiling point (to equilibrium mixture) is 1449 K which agrees with 1443 K reported by Wartenberg and Schulz, and also 1462 K by Ruff and Mugdan.

Reaction	Source	$\Delta_f H^\circ(298.15\text{ K})$ , kcal·mol <sup>-1</sup>
LiI(cr) → LiI(g)	Gorokhov	44.7
	Friedman	43.9
2 LiI(cr) → Li <sub>2</sub> I <sub>2</sub> (g)	Gorokhov	46.0
	Friedman	44.1
Li <sub>2</sub> I <sub>2</sub> (g) → 2 LiI(g)	Berkowitz <i>et al.</i>	38.8
	Friedman	43.7
	Gorokhov	43.2
		42.2
		41.3
		41.3
		43.1

Heat Capacity and Entropy

The bond distance and the rotational constants ( $B_e$  and  $\nu_2$ ), corrected to the isotopic abundance of 7.4% Li<sup>6</sup> and 92.6% Li<sup>7</sup>, were obtained from the microwave studies by Honig *et al.*<sup>8</sup> The vibrational constants ( $\omega_e$  and  $\omega_e x_e$ ) were determined from the infrared spectrum by Klempner *et al.*<sup>9</sup>

The tabulated thermodynamic functions are in reasonable agreement with those calculated by Wilkins who used slightly different molecular constants.

References

- L. N. Gorokhov, Dokl. Akad. Nauk SSSR 142, 113 (1962).
- L. Friedman, J. Chem. Phys. 23, 477 (1955).
- J. Berkowitz, H. A. Tassman and W. A. Chupka, J. Chem. Phys. 36, 2170 (1962).
- O. Ruff and S. Mugdan, Z. Anorg. Chem. 117, 147 (1921).
- H. von Wartenberg and H. Schulz, Z. Elektrochem. 27, 568 (1921).
- A. Honig, M. Mandel, M. L. Stinch and C. H. Townes, Phys. Rev. 96, 629 (1954).
- W. Klempner, W. G. Norris, A. Buchler and A. G. Emslie, J. Chem. Phys. 33, 1534 (1960).
- R. L. Wilkins, J. Chem. Eng. Data 5, 337 (1960).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - R ln(T <sub>r</sub> )]/T <sub>r</sub>	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>f</sub> G <sup>o</sup>	
0	0	0	INFINITE	INFINITE	INFINITE
100	29.475	197.607	-6.383	-89.078	-89.078
200	32.394	218.879	-3.297	-88.184	-88.184
250	33.663	226.251	-1.644	-89.405	-89.405
298.15	34.572	232.262	0	-90.194	-90.194
300	34.602	232.476	0.064	-91.002	-91.002
350	35.289	237.864	1.812	-134.534	-134.534
400	35.798	242.611	3.590	-141.955	-141.955
450	36.185	246.851	5.390	-148.480	-148.480
500	36.485	250.679	7.207	-154.327	-154.327
600	36.921	257.372	10.879	-173.442	-173.442
700	37.223	263.088	14.587	-183.755	-183.755
800	37.448	268.074	18.371	-193.531	-193.531
900	37.627	272.495	22.075	-202.664	-202.664
1000	37.777	276.467	25.845	-211.627	-211.627
1100	37.906	280.074	29.629	-220.431	-220.431
1200	38.022	283.377	33.426	-229.078	-229.078
1300	38.128	286.425	37.234	-237.572	-237.572
1400	38.227	289.254	41.051	-245.917	-245.917
1500	38.321	291.895	44.879	-254.117	-254.117
1600	38.410	294.371	48.715	-262.172	-262.172
1700	38.496	296.705	52.561	-270.089	-270.089
1800	38.580	298.905	56.415	-277.868	-277.868
1900	38.663	300.993	60.277	-285.519	-285.519
2000	38.742	302.978	64.147	-293.044	-293.044
2100	38.821	304.870	68.025	-300.439	-300.439
2200	38.899	306.678	71.911	-307.706	-307.706
2300	38.976	308.409	75.800	-314.843	-314.843
2400	39.052	310.069	79.706	-321.851	-321.851
2500	39.128	311.663	83.615	-328.724	-328.724
2600	39.203	313.201	87.532	-335.464	-335.464
2700	39.277	314.682	91.456	-342.072	-342.072
2800	39.352	316.112	95.387	-348.549	-348.549
2900	39.426	317.494	99.326	-354.894	-354.894
3000	39.499	318.832	103.272	-361.106	-361.106
3100	39.572	320.128	107.226	-367.184	-367.184
3200	39.645	321.386	111.187	-373.128	-373.128
3300	39.718	322.607	115.155	-378.938	-378.938
3400	39.791	323.794	119.131	-384.614	-384.614
3500	39.863	324.948	123.113	-390.156	-390.156
3600	39.936	326.072	127.103	-395.564	-395.564
3700	40.008	327.167	131.100	-400.838	-400.838
3800	40.080	328.233	135.105	-405.978	-405.978
3900	40.152	329.277	139.116	-410.984	-410.984
4000	40.224	330.295	143.135	-415.855	-415.855
4100	40.296	331.289	147.161	-420.592	-420.592
4200	40.368	332.261	151.194	-425.194	-425.194
4300	40.439	333.211	155.232	-429.662	-429.662
4400	40.511	334.142	159.282	-433.994	-433.994
4500	40.583	335.053	163.337	-438.191	-438.191
4600	40.654	335.946	167.399	-442.244	-442.244
4700	40.726	336.821	171.468	-446.154	-446.154
4800	40.797	337.679	175.544	-449.921	-449.921
4900	40.869	338.521	179.627	-453.544	-453.544
5000	40.940	339.347	183.718	-457.021	-457.021
5100	41.011	340.159	187.815	-460.352	-460.352
5200	41.083	340.956	191.920	-463.544	-463.544
5300	41.154	341.739	196.032	-466.594	-466.594
5400	41.225	342.509	200.151	-469.501	-469.501
5500	41.296	343.266	204.277	-472.264	-472.264
5600	41.368	344.011	208.410	-474.891	-474.891
5700	41.439	344.744	212.550	-477.384	-477.384
5800	41.510	345.465	216.698	-479.744	-479.744
5900	41.581	346.175	220.852	-481.971	-481.971
6000	41.652	346.875	225.014	-484.064	-484.064

PREVIOUS: June 1966 (1 atm)

CURRENT: June 1966 (1 bar)

Lithium Iodide (LiI)

$I_2Li_2(g)$

Magnesium Iodide (MgI)

$M_f = 151.2095$

Magnesium Iodide (MgI)

$I_1, Mg(g)$

$S^\circ(298.15\text{ K}) = 252.647 \pm 0.21\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(0\text{ K}) = [26.45 \pm 41.8]\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [24.61 \pm 41.8]\text{ kJ}\cdot\text{mol}^{-1}$

Electronic Levels and Quantum Weights	$g_i$
State	
$X^1\Sigma^+$	0
$A^1\Pi$	24319
	25294

$\omega_e = 312\text{ cm}^{-1}$   
 $B_e = [0.13014]\text{ cm}^{-1}$   
 $\omega_e x_e = [1.09]\text{ cm}^{-1}$   
 $\alpha_e = [0.00062]\text{ cm}^{-1}$   
 $\sigma = 1$   
 $r_e = [2.52]\text{ \AA}$

Enthalpy of Formation

The adopted  $\Delta_f H^\circ(0\text{ K}) = 6.309 \pm 10\text{ kcal}\cdot\text{mol}^{-1}$  is calculated from a  $D_0$  value of  $54.3\text{ kcal}\cdot\text{mol}^{-1}$  ( $2.35\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ ). An approximate value of  $312\text{ cm}^{-1}$  has been given for  $\omega_e$ . A value of  $\omega_e x_e = 1.09\text{ cm}^{-1}$  is calculated from an average value of  $x_e \mu^{1/2}$  calculated from data for CaI, SrI, BaI, MgBr, and MgCl.<sup>1,2</sup> A linear Birge-Sponner extrapolation of these  $\omega_e$  and  $\omega_e x_e$  data is corrected for the ionic character of the molecule as described by Hildenbrand to give the adopted value of  $D_0 = 54.3\text{ kcal}\cdot\text{mol}^{-1}$ .

From a consideration of ionic bonding forces, Krasnov and Karaseva<sup>3</sup> calculated  $D_0 \approx 55 \pm 10\text{ kcal}\cdot\text{mol}^{-1}$ . Using JANAF data,  $D_0(\text{MgI}) = 0.44$ , in reasonable agreement with the ratios found by Blue *et al.*<sup>4</sup> for the alkali earth fluorides and by Hildenbrand for the alkaline with fluorides and chlorides.

$\Delta_f H^\circ(298.15\text{ K}) = 5.883 \pm 10\text{ kcal}\cdot\text{mol}^{-1}$  is calculated from the adopted  $\Delta_f H^\circ(0\text{ K}) = 6.309\text{ kcal}\cdot\text{mol}^{-1}$ .

Heat Capacity and Entropy

The ground state vibrational constants are as given in the Enthalpy of Formation section above. The adopted value of  $r_e = 2.52\text{ \AA}$  is the bond distance in  $\text{MgI}_2$ .<sup>5</sup> Margrave<sup>6</sup> has estimated  $2.72\text{ \AA}$  from additive ionic radii.  $B_e$  is calculated from the adopted  $r_e$ , and  $\alpha_e$  is calculated assuming a Morse potential function.

The electronic levels and their designation are those given by Rosen.<sup>1</sup> The possibility of additional electronic levels near  $15000\text{ cm}^{-1}$  is suggested by a comparison with CaI, SrI, and BaI<sup>2</sup> including these levels does not change the entropy at  $298.15\text{ K}$  and increases the entropy at  $6000\text{ K}$  by only  $0.69\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ .

References

- B. Rosen, Ed. "Spectroscopic Data Relative to Diatomic Molecules," Pergamon Press, New York, (1970).
- JANAF Thermochemical Tables: CaI(g), SrI(g), BaI(g), 6-30-74; MgBr(g), 6-30-66; MgCl(g) 3-31-66.
- D. L. Hildenbrand in "Advances in High Temperature Chemistry," Vol. 1, L. Eyring, Ed., Academic Press, New York, pp 193-215, (1967).
- K. S. Krasnov and N. V. Karaseva, Optics and Spectroscopy, 19, 14 (1965).
- G. D. Blue, J. W. Green, T. C. Ehler, and J. L. Margrave, Nature 199, 804 (1963).
- D. L. Hildenbrand, Stanford Research Institute, personal communication, (July 2, 1974).
- P. A. Akishin and V. P. Spiridonov, Zhur Fiz. Khim 32, 1682 (1958).
- J. L. Margrave, J. Phys. Chem. 58, 258 (1954).

T/K	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $P^\circ = 0.1\text{ MPa}$		log K <sub>r</sub>
	$C_p^\circ$	$S^\circ - (G^\circ - H^\circ(T_r))/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	
0	0	INFINITE	-9.765	26.446	INFINITE
100	31.085	215.601	-6.811	27.233	-5.053
200	34.773	238.459	-3.492	26.079	-7.488
250	35.645	246.320	-1.730	25.356	-15.798
298.15	36.178	252.647	0	24.614	-23.658
300	36.195	252.871	0.087	24.585	-23.957
350	36.562	258.480	1.886	23.736	-31.982
400	36.821	263.380	3.721	14.865	-39.608
450	37.013	267.728	5.567	13.374	-46.327
500	37.160	271.636	7.422	-8.199	-50.980
600	37.376	278.431	11.419	-9.116	-59.452
700	37.530	284.203	14.895	-10.126	-67.763
800	37.651	289.224	18.654	-11.245	-75.972
900	37.751	293.665	22.425	-12.488	-83.933
1000	37.840	297.647	26.204	-13.846	-91.686
1100	37.920	301.257	29.992	-15.316	-99.273
1200	37.994	304.560	33.788	-16.894	-106.719
1300	38.064	307.604	37.588	-18.572	-114.034
1400	38.132	310.427	41.391	-20.350	-121.268
1500	38.197	313.060	45.217	-23.223	-128.452
1600	38.261	315.528	49.040	-26.197	-135.587
1700	38.324	317.849	52.869	-29.272	-142.683
1800	38.385	320.041	56.705	-32.446	-149.739
1900	38.446	322.118	60.546	-35.718	-156.765
2000	38.506	324.092	64.394	-39.090	-163.772
2100	38.565	325.972	68.247	-42.562	-170.760
2200	38.623	327.768	72.107	-46.135	-177.730
2300	38.680	329.486	75.972	-49.808	-184.683
2400	38.737	331.133	79.844	-53.580	-191.618
2500	38.802	332.716	83.721	-57.451	-198.530
2600	38.861	334.239	87.604	-61.422	-205.420
2700	38.921	335.703	91.493	-65.493	-212.290
2800	38.981	337.123	95.388	-69.664	-219.140
2900	39.042	338.492	99.289	-73.935	-225.970
3000	39.104	339.817	103.197	-78.306	-232.780
3100	39.168	341.100	107.110	-82.777	-239.570
3200	39.232	342.345	111.030	-87.348	-246.340
3300	39.299	343.553	114.957	-92.019	-253.090
3400	39.368	344.727	118.890	-96.790	-259.820
3500	39.439	345.869	122.831	-101.661	-266.530
3600	39.512	346.982	126.778	-106.632	-273.220
3700	39.588	348.065	130.733	-111.703	-279.890
3800	39.667	349.122	134.696	-116.874	-286.540
3900	39.750	350.153	138.667	-122.145	-293.170
4000	39.835	351.161	142.646	-127.516	-299.780
4100	39.925	352.146	146.634	-132.987	-306.370
4200	40.017	353.109	150.631	-138.558	-312.940
4300	40.114	354.052	154.637	-144.229	-319.480
4400	40.214	354.975	158.654	-150.000	-326.000
4500	40.318	355.880	162.680	-155.871	-332.500
4600	40.427	356.767	166.718	-161.842	-339.000
4700	40.539	357.638	170.766	-167.913	-345.490
4800	40.654	358.492	174.826	-174.084	-351.970
4900	40.774	359.332	178.897	-180.355	-358.440
5000	40.897	360.157	182.980	-186.726	-364.900
5100	41.024	360.968	187.076	-193.197	-371.350
5200	41.155	361.766	191.185	-199.768	-377.790
5300	41.289	362.551	195.308	-206.439	-384.220
5400	41.427	363.324	199.443	-213.210	-390.640
5500	41.567	364.086	203.593	-220.081	-397.050
5600	41.711	364.836	207.757	-227.052	-403.450
5700	41.857	365.575	211.935	-234.123	-409.840
5800	42.006	366.305	216.128	-241.294	-416.220
5900	42.158	367.024	220.337	-248.565	-422.590
6000	42.312	367.734	224.560	-255.936	-429.000

PREVIOUS: December 1974 (1 atm)

CURRENT: December 1974 (1 bar)

Magnesium Iodide (MgI)

$I_1, Mg(g)$

IDEAL GAS

Molybdenum Iodide (Mol)

M<sub>r</sub> = 222.8445 Molybdenum Iodide (Mol)

I<sub>2</sub>Mo<sub>2</sub>(g)

S°(298.15 K) = [278.974 ± 8.4] J·K<sup>-1</sup>·mol<sup>-1</sup> ΔH<sup>0</sup>(0 K) = [499.74 ± 41.8] kJ·mol<sup>-1</sup> ΔH<sup>0</sup>(298.15 K) = [498.73 ± 41.8] kJ·mol<sup>-1</sup>

Electronic Levels and Quantum Weights			
ε <sub>e</sub> , cm <sup>-1</sup>	g <sub>e</sub>	ε <sub>e</sub> , cm <sup>-1</sup>	g <sub>e</sub>
0	[6]	[15199]	[6]
[11783]	[2]	[15331]	[8]
[12034]	[4]	[15428]	[10]
[12417]	[6]	[16947]	[8]
[12900]	[8]	[17174]	[4]
[13461]	[10]	[17344]	[6]
		[15699]	[4]

ω<sub>e</sub> = [200] cm<sup>-1</sup> ω<sub>e</sub>x<sub>e</sub> = [0.41] cm<sup>-1</sup> σ = 1  
 B<sub>e</sub> = [0.04361] cm<sup>-1</sup> α<sub>e</sub> = [0.00013] cm<sup>-1</sup> r<sub>e</sub> = [2.66] Å

Enthalpy of Formation

The adopted value of ΔH<sup>0</sup> at 298.15 K is that estimated by Brewer.<sup>1</sup> The estimated value is consistent with the low volatility of solid molybdenum in iodine vapor reported by Schafer *et al.*<sup>2</sup> Brewer's estimated value is given as ΔH<sup>0</sup>(298.15 K)R = 60000 ± 5000. The assigned uncertainty (±10 kcal·mol<sup>-1</sup>) is determined from the product 500 × R which has been rounded to the nearest kcal·mol<sup>-1</sup>. The value of ΔH<sup>0</sup>(0 K) combined with JANAF data<sup>3</sup> for Mo(g) and I(g) gives D<sup>0</sup>(Mo-I) = 63 ± 11 kcal·mol<sup>-1</sup>.

Heat Capacity and Entropy

We use values of r<sub>e</sub> and ω<sub>e</sub> estimated by Brewer.<sup>1</sup> The electronic contribution is taken to be the same as that for the free gaseous Mo<sup>0</sup> ion, as suggested by Brewer.<sup>1</sup> The levels listed by Moore<sup>4</sup> below 17334 cm<sup>-1</sup> are used in the calculations. Our thermodynamic functions differ slightly from those reported by Brewer<sup>1</sup> due to the use of non-zero values for ω<sub>e</sub>x<sub>e</sub> and α<sub>e</sub>. Estimates for α<sub>e</sub> and ω<sub>e</sub> are based on the empirical correlations of Calder and Ruedenberg.<sup>5</sup>

References

- L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal communication; September 28, 1978, preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria.
- H. Schafer, T. Grofe, and M. Trenkel, *J. Solid State Chem.* 8, 14 (1973).
- JANAF Thermochemical Tables: Mo(g), 3-31-78; I(g) and Si(g), 6-30-74.
- C. E. Moore, NSRDS NBS 34, 1970; NSRDS NBS 35, Vol. III, Reissued (1971).
- G. V. Calder and K. Ruedenberg, *J. Chem. Phys.* 49, 5399 (1968).

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ))/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	ΔH <sup>o</sup>	Standard State Pressure = P <sup>o</sup> = 0.1 MPa	log K <sub>r</sub>
0	0.	INFINITE	-10.173	499.744	499.744	INFINITE
100	33.511	240.056	-7.118	500.783	480.529	-251.073
200	36.229	264.348	-3.598	499.994	460.516	-120.204
250	36.692	272.487	-1.774	499.386	450.715	-94.172
298.15	36.962	278.974	0.	498.733	441.399	-77.331
300	36.970	279.203	0.068	498.707	441.043	-76.792
350	37.154	284.917	1.922	497.940	431.492	-64.397
400	37.285	289.887	3.783	489.146	422.328	-55.150
450	37.384	294.284	5.650	487.732	414.060	-48.063
500	37.463	298.227	7.521	485.851	407.851	-42.608
600	37.586	305.069	11.274	465.497	396.242	-34.496
700	37.682	310.870	15.037	464.704	384.762	-28.711
800	37.757	315.907	18.810	463.865	373.398	-24.380
900	37.837	320.360	22.590	462.984	362.142	-21.018
1000	37.905	324.350	26.377	462.057	350.987	-18.334
1100	37.970	327.966	30.058	461.081	339.926	-16.142
1200	38.035	331.272	33.971	460.046	328.958	-14.319
1300	38.100	334.319	37.778	458.944	318.078	-12.781
1400	38.170	337.145	41.591	457.764	307.286	-11.465
1500	38.249	339.781	45.412	456.496	296.581	-10.236
1600	38.342	342.253	49.241	455.130	285.964	-9.036
1700	38.456	344.580	53.081	453.656	275.436	-8.463
1800	38.599	346.782	56.933	452.067	264.997	-7.690
1900	38.780	348.874	60.802	450.356	254.651	-7.001
2000	39.007	350.869	64.691	448.518	244.397	-6.383
2100	39.288	352.778	68.605	446.552	234.239	-5.826
2200	39.630	354.614	72.550	444.456	224.177	-5.323
2300	40.040	356.384	76.533	442.232	214.214	-4.865
2400	40.523	358.098	80.561	439.881	204.351	-4.448
2500	41.082	359.763	84.650	437.405	194.587	-4.066
2600	41.718	361.387	88.780	434.796	184.925	-3.715
2700	42.430	362.974	92.967	432.027	175.367	-3.393
2800	43.218	364.531	97.268	429.050	165.915	-3.095
2900	44.075	366.063	101.632	425.819	156.623	-2.821
3000	44.997	367.572	106.086	422.347	148.605	-2.587
3100	45.975	369.064	110.634	418.693	140.638	-2.370
3200	47.001	370.539	115.282	414.351	132.716	-2.166
3300	48.065	372.002	120.035	409.584	124.834	-1.976
3400	49.156	373.453	124.896	404.408	116.986	-1.797
3500	50.263	374.894	129.867	398.830	109.168	-1.629
3600	51.375	376.325	134.949	392.859	101.375	-1.471
3700	52.481	377.748	140.142	386.485	93.603	-1.321
3800	53.568	379.162	145.444	380.341	85.946	-1.180
3900	54.628	380.567	150.854	373.955	78.102	-1.046
4000	55.649	381.963	156.369	367.702	70.366	-0.919
4100	56.625	383.350	161.983	361.584	62.834	-0.798
4200	57.546	384.725	167.692	355.599	55.404	-0.683
4300	58.407	386.090	173.490	349.728	47.172	-0.573
4400	59.202	387.441	179.371	343.968	39.437	-0.468
4500	59.928	388.780	185.328	338.261	31.695	-0.368
4600	60.581	390.105	191.354	332.689	23.944	-0.272
4700	61.161	391.414	197.442	327.246	16.183	-0.180
4800	61.665	392.707	203.584	321.931	8.411	-0.092
4900	62.096	393.983	209.772	316.742	0.625	-0.007
5000	62.454	395.241	216.001	311.678	-1.144	0.015
5100	62.742	396.481	222.261	306.742	-1.908	0.028
5200	62.961	397.701	228.547	301.933	-2.662	0.069
5300	63.116	398.902	234.851	297.252	-3.404	0.109
5400	63.210	400.083	241.168	292.702	-4.134	0.148
5500	63.247	401.243	247.491	288.281	-4.854	0.185
5600	63.231	402.383	253.815	283.992	-5.564	0.221
5700	63.166	403.502	260.136	279.836	-6.264	0.257
5800	63.057	404.599	266.447	275.814	-6.954	0.291
5900	62.908	405.676	272.746	271.927	-7.634	0.325
6000	62.723	406.732	279.028	268.174	-8.304	0.357

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

Molybdenum Iodide (Mol)

I<sub>2</sub>Mo<sub>2</sub>(g)

Nitrosyl Iodide (NOI)

$$S^{\circ}(298.15\text{ K}) = [282.960] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$\Delta H^{\circ}(0\text{ K}) = [115.30 \pm 20.9] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta H^{\circ}(298.15\text{ K}) = [112.13 \pm 20.9] \text{ kJ}\cdot\text{mol}^{-1}$$

IDEAL GAS

Vibrational Frequencies and Degeneracies

$\nu$ , $\text{cm}^{-1}$
[1780](1)
[440](1)
[200](1)

Ground State Quantum Weight: 1

Point Group:  $C_{2v}$

Bond Distances: O-N = [1.15] Å N-I = [2.3] Å

Bond Angle: O-N-I = [120]°

Product of the Moments of Inertia:  $I_A I_B I_C = [7.908120 \times 10^{11}] \text{ g}^3\cdot\text{cm}^6$

$\alpha = 1$

Enthalpy of Formation

The enthalpy of formation  $\Delta H^{\circ}(298.15\text{ K})$  for  $\text{INO}(\text{g})$  is estimated by comparison with those for  $\text{FNO}(\text{g})$ ,  $\text{ClNO}(\text{g})$ ,  $\text{BrNO}(\text{g})$ , and the related cyanogen halides.

Heat Capacity and Entropy

The molecular structure and bond angle are estimated by comparison with those for  $\text{ClNO}(\text{g})$  and  $\text{BrNO}(\text{g})$ . The N-O bond distance is assumed to be the same as that in  $\text{NO}(\text{g})$ . The N-I bond distance,  $r(\text{N-I})$  is calculated based on an assumption that  $r(\text{ON-Cl})/r(\text{ON-I}) = r(\text{Cl-Cl})/r(\text{I-I})$ . The vibrational frequencies are estimated by comparison with those for  $\text{FNO}(\text{g})$ ,  $\text{ClNO}(\text{g})$  and  $\text{BrNO}(\text{g})$ . The three principal moments of inertia are:  $I_A = 0.8962 \times 10^{-39}$ ,  $I_B = 29.2605 \times 10^{-39}$ , and  $I_C = 30.1568 \times 10^{-39} \text{ g}\cdot\text{cm}^2$ .

Nitrosyl Iodide (ONI)

$$M_r = 156.9106$$



T/K	$C_p^{\circ}$	$S^{\circ} - [C_p^{\circ} - H^{\circ}(T)]/T$	$H^{\circ} - H^{\circ}(T)$	$\Delta H^{\circ}$	$\Delta G^{\circ}$	log K <sub>r</sub>
Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$						
Standard State Pressure = $p^{\circ} = 0.1\text{ MPa}$						
Units: $\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , $\text{kJ}\cdot\text{mol}^{-1}$						
0	0	0	0	0	0	INFINITE
100	38.203	236.247	322.541	-8.629	110.430	-57.683
200	44.111	264.773	287.171	-4.480	107.010	-72.948
250	45.744	274.803	283.726	-2.231	105.543	-72.052
298.15	46.836	282.960	282.960	0	104.227	-18.260
300	46.893	283.250	282.961	0.087	104.178	-18.139
350	47.790	290.548	283.535	2.455	102.894	-15.356
400	48.566	296.981	284.822	4.864	101.314	-13.314
450	49.279	302.743	286.498	7.310	101.875	-11.825
500	49.950	307.970	288.388	9.791	102.065	-10.845
600	51.181	317.188	292.440	14.849	108.371	-9.435
700	52.248	325.169	296.558	20.072	112.091	-8.423
800	53.146	332.197	300.581	25.293	117.429	-7.662
900	53.890	338.501	304.451	30.646	121.977	-7.076
1000	54.503	344.212	308.146	36.066	126.407	-6.603
1100	55.006	349.431	311.665	41.543	130.869	-6.214
1200	55.422	354.236	315.015	47.065	135.317	-5.890
1300	55.767	358.686	318.205	52.625	139.752	-5.615
1400	56.055	362.829	321.246	58.216	144.177	-5.379
1500	56.297	366.705	324.149	63.834	148.594	-5.174
1600	56.502	370.345	326.924	69.474	153.005	-4.995
1700	56.677	373.776	329.580	75.133	157.413	-4.837
1800	56.827	377.020	332.126	80.809	161.820	-4.696
1900	56.956	380.096	334.571	86.498	166.229	-4.570
2000	57.069	383.020	336.921	92.199	170.641	-4.457
2100	57.167	385.807	339.183	97.911	175.059	-4.354
2200	57.253	388.469	341.363	103.627	179.486	-4.262
2300	57.329	391.015	343.467	109.352	183.920	-4.177
2400	57.397	393.457	345.499	115.098	188.365	-4.100
2500	57.457	395.801	347.465	120.841	192.820	-4.029
2600	57.511	398.056	349.367	126.589	197.288	-3.964
2700	57.559	400.227	351.211	132.343	201.767	-3.903
2800	57.602	402.321	352.999	138.101	206.258	-3.848
2900	57.641	404.343	354.735	143.863	210.759	-3.796
3000	57.677	406.298	356.422	149.629	215.273	-3.748
3100	57.709	408.190	358.061	155.398	219.797	-3.704
3200	57.738	410.022	359.656	161.171	224.331	-3.662
3300	57.765	411.799	361.210	166.946	228.875	-3.623
3400	57.790	413.524	362.723	172.724	233.427	-3.586
3500	57.812	415.200	364.199	178.504	237.988	-3.552
3600	57.833	416.829	365.638	184.286	242.555	-3.519
3700	57.852	418.414	367.043	190.070	247.129	-3.489
3800	57.870	419.957	368.415	195.856	251.710	-3.460
3900	57.886	421.460	369.756	201.644	256.295	-3.433
4000	57.902	422.926	371.067	207.434	260.884	-3.407
4100	57.916	424.356	372.350	213.225	265.476	-3.382
4200	57.929	425.751	373.605	219.017	270.072	-3.359
4300	57.941	427.115	374.833	224.810	274.671	-3.337
4400	57.953	428.447	376.037	230.605	279.270	-3.315
4500	57.964	429.749	377.216	236.401	283.872	-3.295
4600	57.974	431.023	378.372	242.198	288.474	-3.276
4700	57.983	432.270	379.505	247.996	293.076	-3.257
4800	57.992	433.491	380.617	253.794	297.679	-3.239
4900	58.000	434.687	381.709	259.594	302.282	-3.222
5000	58.008	435.859	382.780	265.394	306.883	-3.206
5100	58.015	437.008	383.832	271.195	311.484	-3.190
5200	58.022	438.134	384.866	276.997	316.083	-3.175
5300	58.029	439.240	385.881	282.800	320.681	-3.160
5400	58.035	440.324	386.879	288.603	325.277	-3.146
5500	58.041	441.389	387.861	294.407	329.871	-3.133
5600	58.047	442.435	388.826	300.211	334.464	-3.120
5700	58.052	443.463	389.775	306.016	339.054	-3.107
5800	58.057	444.472	390.710	311.822	343.642	-3.095
5900	58.062	445.465	391.628	317.628	348.228	-3.083
6000	58.066	446.441	392.535	323.434	352.812	-3.072

PREVIOUS: December 1966 (1 atm)

CURRENT: December 1966 (1 bar)

Nitrosyl Iodide (ONI)



Sodium Iodide (NaI) CRYSTAL

$M_r = 149.89427$  Sodium Iodide (NaI)

$I_1Na_1(cr)$

$S^\circ(298.15\text{ K}) = 98.500\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{fus} = 933\text{ K}$   
 $\Delta H_f^\circ(0\text{ K}) = -287.34 \pm 0.8\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = -287.86 \pm 0.8\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{fus} H^\circ = 23.598\text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation

The enthalpy of formation was obtained as follows:

- (1)  $HI \cdot 100H_2O + NaOH \cdot 100H_2O \rightarrow NaI \cdot 201H_2O$
  - (2)  $Na(cr) + 100H_2O(l) \rightarrow NaOH \cdot 1000H_2O + 1/2H_2(g)$
  - (3)  $NaOH \cdot 1000H_2O \rightarrow NaOH \cdot 100H_2O + 900H_2O(l)$
  - (4)  $1/2H_2(g) + 1/2I_2(s) \rightarrow HI(g)$
  - (5)  $HI(g) + 100H_2O(l) \rightarrow HI \cdot 100H_2O$
  - (6)  $NaI \cdot 201H_2O(l) \rightarrow NaI(cr) + 201\text{ H}_2\text{O}(l)$
- (1) + (2) + (3) + (4) + (5) + (6) gives  $Na(cr) + 1/2I_2(s) \rightarrow NaI(cr)$

Heat Capacity and Entropy

Smoothed heat capacities between 3 and 270 K have been presented by Berg and Morrison.<sup>9</sup> Above 270 K the heat capacity was obtained by comparing with  $KI(cr)$  on a reduced temperature plot of  $C_p/T$  versus  $T$ . The values so obtained were increased by 1.4% to bring them into line with the low temperature data.

Fusion Data

Dworkin and Bredig<sup>10</sup> have measured both  $T_{fus}$  and  $\Delta_{fus}H$ .

References

- <sup>1</sup>T. W. Richards and A. W. Rowe, *J. Amer. Chem. Soc.* **44**, 684 (1922).
- <sup>2</sup>S. R. Gunn and L. G. Green, *J. Amer. Chem. Soc.* **80**, 4782 (1958).
- <sup>3</sup>U. S. Nat. Bur. Stand. Circ. 500, 1268 pp. (1952).
- <sup>4</sup>JANAF Thermochemical Tables.
- <sup>5</sup>W. A. Roth, *Z. Elektrochem.* **50**, 107 (1944).
- <sup>6</sup>J. Wust and E. Lange, *Z. Physik. Chem.* **116**, 161 (1925).
- <sup>7</sup>E. Lange and A. L. Robinson, *Chem. Revs.* **9**, 89 (1931).
- <sup>8</sup>Askew, Bullock, Smith, Tinkler, Gatty and Wollenden, *J. Chem. Soc.*, 1368 (1934).
- <sup>9</sup>W. T. Berg and J. A. Morrison, *Proc. Roy. Soc. (London)* **242A**, 467 (1957).
- <sup>10</sup>A. Dworkin and M. Bredig, *J. Phys. Chem.* **64**, 269 (1960).

T/K	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$		log $K_r$
	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	
0	0	INFINITE	-12.523	-287.336	INFINITE
100	43.032	143.089	-9.749	-286.556	149.681
200	49.852	78.103	-5.021	-285.606	74.593
298.15	52.225	98.500	0	-284.572	49.856
300	52.258	98.823	0.097	-284.551	49.543
400	53.806	114.077	5.403	-282.898	36.943
500	55.020	126.213	10.844	-276.772	28.914
600	56.233	136.353	16.407	-268.035	23.335
700	57.363	145.106	22.087	-259.404	19.358
800	58.492	152.840	27.880	-250.945	16.385
900	59.580	159.793	33.784	-242.598	14.080
933.000	59.939	161.945	35.756	--- CRYSTAL $\leftarrow$ --- LIQUID	---
1000	60.675	166.127	39.796	-315.904	12.243
1100	61.764	171.961	45.918	-314.598	10.746
1200	62.844	177.381	52.149	-409.994	9.397
1300	63.914	182.454	58.487	-407.663	8.078
1400	64.974	187.279	64.931	-405.241	6.861
1500	66.024	191.748	71.481	-402.733	5.857
1600	67.064	195.042	78.136	-400.146	4.983
1700	68.093	200.139	84.894	-397.484	4.217
1800	69.116	204.060	91.754	-394.753	3.541
1900	70.127	207.824	98.717	-391.956	2.940
2000	71.128	211.446	105.779	-389.093	2.403

PREVIOUS

CURRENT: September 1963

Sodium Iodide (NaI)

$I_1Na_1(cr)$

Sodium Iodide (NaI)  $I_1Na_1(I)$  $M_r = 149.89427$ 

LIQUID

$$S^\circ(298.15 \text{ K}) = [120.754] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$$

$$T_{\text{fus}} = 933 \text{ K}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = [-266.508] \text{ kJ}\cdot\text{mol}^{-1}$$

$$\Delta_{\text{sub}} H^\circ = 23\,598 \text{ kJ}\cdot\text{mol}^{-1}$$

## Enthalpy of Formation

$\Delta_f H^\circ(\text{NaI}, l, 298.15 \text{ K})$  is calculated from that of the crystal by adding  $\Delta_{\text{sub}} H^\circ$  and the difference in enthalpy,  $H^\circ(933 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and liquid.

## Heat Capacity and Entropy

$C_p^\circ$  is estimated assuming each atom contributed 7.75  $\text{cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ .  $S^\circ(\text{NaI}, l, 298.15 \text{ K})$  is calculated in a manner similar to that used for the enthalpy of formation.

## Fusion Data

Refer to the crystal table for details.

## Vaporization Data

The boiling point,  $T_{\text{vap}} = 1577 \text{ K}$  ( $l \rightarrow$  equilibrium mixture, 1 atm), is that given by Kelley<sup>1</sup> from examination of the high temperature vapor pressure.

## Reference

<sup>1</sup>K. K. Kelley, U. S. Bur. of Mines Bull. 383, (1935).

T/K	$C_p^\circ$	Enthalpy Reference Temperature = $T_r = 298.15 \text{ K}$		Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$		$I_1Na_1(I)$
		$S^\circ$	$-(G^\circ - H^\circ(T_r))/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f G^\circ$	
0						
100						
200						
298.15	52.225	120.754	120.754	0.	-266.508	47.278
300	52.258	121.077	120.755	0.097	-266.514	46.990
400	53.806	136.331	122.824	5.403	-277.649	35.317
500	55.020	148.468	126.780	10.844	-299.407	27.846
600	56.233	158.606	131.262	16.407	-298.737	22.638
600.000	56.233	158.606	131.262	16.407		
600.000	64.852	158.606	131.262	16.407		
700	64.852	168.603	135.901	22.892	-297.088	18.933
800	64.852	177.263	140.543	29.377	-295.401	16.169
900	64.852	184.902	143.055	35.862	-293.699	14.032
933.000	64.852	187.237	146.506	38.002		
1000	64.852	191.734	149.387	42.347	-292.002	12.332
1100	64.852	197.915	153.522	48.833	-290.333	10.949
1200	64.852	203.558	157.460	55.318	-385.474	9.697
1300	64.852	208.749	161.208	61.803	-382.995	8.411
1400	64.852	213.555	164.778	68.288	-380.532	7.315
1500	64.852	218.030	168.181	74.773	-378.089	6.371
1600	64.852	222.215	171.428	81.259	-375.672	5.551
1700	64.852	226.147	174.533	87.744	-373.283	4.832
1800	64.852	229.854	177.504	94.229	-370.927	4.196
1900	64.852	233.360	180.352	100.714	-368.607	3.632
2000	64.852	236.686	183.087	107.199	-366.322	3.127
2100	64.852	239.851	185.715	113.685	-364.071	2.672
2200	64.852	242.867	188.245	120.170	-361.854	2.262
2300	64.852	245.750	190.683	126.655	-359.666	1.890
2400	64.852	248.510	193.035	133.140	-357.503	1.550
2500	64.852	251.158	195.308	139.625	-355.360	1.240
2600	64.852	253.701	197.505	146.111	-353.233	0.955
2700	64.852	256.140	199.632	152.596	-351.116	0.693
2800	64.852	258.507	201.693	159.081	-349.005	0.451
2900	64.852	260.783	203.691	165.566	-346.897	0.227
3000	64.852	262.982	205.611	172.051	-344.787	0.020

PREVIOUS:

CURRENT: September 1963

## Sodium Iodide (NaI)

 $I_1Na_1(I)$



Sodium Iodide (NaI)

CRYSTAL-LIQUID

0 to 933 K crystal  
above 933 K liquid

Refer to the individual tables for details.

$M_r = 149.89427$  Sodium Iodide (NaI)

$I_1Na_1(cr,l)$

T/K	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa		log $K_r$
	$C_p^\circ$	$S^\circ - (G^\circ - H^\circ(T_r))/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	
0	0	0	INFINITE	INFINITE	INFINITE
100	43.032	45.601	143.089	-287.336	-287.336
200	49.852	78.103	103.207	-287.477	-286.556
298.15	52.225	98.500	98.500	-287.621	-285.606
300	52.258	98.501	98.501	-287.659	-284.572
400	53.806	114.077	100.570	-287.865	-284.551
500	55.020	126.213	104.526	-289.000	-282.898
600	56.233	136.353	109.008	-320.758	-276.772
700	57.563	145.106	113.554	-320.088	-268.035
800	58.492	152.840	117.990	-319.244	-259.424
900	59.580	159.793	122.255	-318.250	-250.945
933.000	59.939	161.945	123.621	-317.128	-242.598
933.000	64.852	187.237	123.621	35.756	CRYSTAL $\leftarrow$ LIQUID TRANSITION
1000	64.852	191.734	128.036	59.354	292.002
1100	64.852	197.915	134.112	63.699	-236.087
1200	64.852	203.538	139.667	70.184	-290.333
1300	64.852	208.749	144.784	76.669	-385.474
1400	64.852	213.555	149.527	83.154	-222.776
1500	64.852	218.030	153.946	89.639	-382.995
1600	64.852	222.215	158.084	96.125	-209.318
1700	64.852	226.147	161.973	102.610	-196.051
1800	64.852	229.854	165.642	109.095	-378.089
1900	64.852	233.360	169.115	115.580	-170.030
2000	64.852	236.686	172.411	122.065	-157.250
2100	64.852	239.850	175.548	128.551	-144.611
2200	64.852	242.867	178.540	135.036	-132.101
2300	64.852	245.750	181.400	141.521	-119.713
2400	64.852	248.510	184.139	148.006	-366.322
2500	64.852	251.158	186.767	154.491	-119.713
2600	64.852	253.701	189.293	160.977	-107.438
2700	64.852	256.149	191.724	167.462	-95.269
2800	64.852	258.507	194.067	173.947	-83.266
2900	64.852	260.783	196.329	180.432	-71.227
3000	64.852	262.982	198.514	186.917	-59.343
				193.403	-47.544
				198.514	-35.116
				203.538	-24.188
				208.749	-12.625
				213.555	0.451
				218.030	12.625
				222.215	24.188
				226.147	35.116
				229.854	47.544
				233.360	60.955
				236.686	74.188
				239.850	87.411
				242.867	100.644
				245.750	113.877
				248.510	127.110
				251.158	140.343
				253.701	153.576
				256.149	166.809
				258.507	180.042
				260.783	193.275
				262.982	206.508

PREVIOUS:

CURRENT: September 1963

Sodium Iodide (NaI)

$I_1Na_1(cr,l)$

I<sub>2</sub>O(g)

Iodine Oxide IO(g)

M<sub>r</sub> = 142.90387

IDEAL GAS

Iodine Oxide (IO)

$D_0^{\circ} = 18892 \pm 1500 \text{ cm}^{-1}$   
 $S^{\circ}(298.15 \text{ K}) = 239.6 \pm 1 \text{ J K}^{-1} \text{ mol}^{-1}$

$\Delta H_f^{\circ}(0 \text{ K}) = 128 \pm 18 \text{ kJ mol}^{-1}$   
 $\Delta H_f^{\circ}(298.15 \text{ K}) = 126 \pm 18 \text{ kJ mol}^{-1}$

State	$T_e$	$g_e$	$\omega_e$	$\omega_e x_e$	$B_e$	$\alpha_e$	$D_e \cdot 10^6$	$r_e/\text{\AA}$
X <sup>2</sup> Π <sub>1/2</sub>	0	2	681.6004	4.3699	0.340206	0.0026296	3.6	1.8676
X <sup>2</sup> Π <sub>1/2</sub>	2091	2	681.6004	4.3699	0.340206	0.0026296	3.6	1.8676
A <sup>1</sup> Π <sub>1/2</sub>	21557.81	2	514.57	5.52	0.27635	0.00273	[3.2]	2.0723
A <sup>1</sup> Π <sub>1/2</sub>	[24698]	2	514.57	5.52	0.27635	0.00273	[3.2]	2.0723

Point Group: C<sub>2v</sub>

## Enthalpy of Formation

The dissociation energy has been calculated by many different techniques. The derived values range from 176 to 250 kJ mol<sup>-1</sup>. The values may be grouped into two types: (1) derived from a treatment of the observed vibrational energy levels and (2) extracted from kinetic studies. The two existing spectroscopic studies by Coleman *et al.*<sup>1</sup> and Durie and Ramsay<sup>2</sup> yield dissociation energy values for IO(g). One should note that the first bound excited state A<sup>2</sup>Π of IO(g) dissociates into [(<sup>2</sup>P<sub>3/2</sub>) + O(<sup>3</sup>D<sub>2</sub>)]. Coleman *et al.*<sup>1</sup> from their study of the IO spectrum in flames, used a graphical Birge-Sponner technique to give 1.92 ± 0.2 eV (185 ± 19 kJ mol<sup>-1</sup>). Durie and Ramsay<sup>2</sup> stated that since only six bands were observed in their study of the absorption spectrum of IO, it was not possible to obtain an accurate value for the dissociation of the ground state. They derived an upper limit of <21976 cm<sup>-1</sup> (2.72 eV or 262.9 kJ mol<sup>-1</sup>) from the observed predissociation Durie and Ramsay felt that a better estimate could be obtained from a Birge-Sponner extrapolation of the first four vibrational levels in the upper state leading to D<sub>0</sub><sup>°</sup> = 10200 cm<sup>-1</sup> for the excited state. However, since the accepted values (at that time, 1958) for ClO and BrO were approximately 10% less than the values calculated by the same procedure, they applied the same correction to IO and calculated 14800 ± 1800 cm<sup>-1</sup> (1.8 ± 0.2 eV or 175.7 ± 21 kJ mol<sup>-1</sup>).

Using flame photometry, Phillips and Sugden<sup>3</sup> measured the intensity of the (0,4) band of IO at 5307 to determine the temperature dependent (1900–2700 K) equilibrium constant for the dissociation energy of IO and obtained D<sub>0</sub><sup>°</sup> = 238.5 ± 25 kJ mol<sup>-1</sup>. This value was calculated from the assumed enthalpy of formation value (relative to the monoatomic gases) of 263.6 kJ mol<sup>-1</sup> at 2000 K and is considerably higher than the earlier determined spectroscopic values. Using current thermal functions and auxiliary data we calculate D<sub>0</sub><sup>°</sup> = 256 kJ mol<sup>-1</sup> or 21400 cm<sup>-1</sup>.

Herron and Huie<sup>4</sup> and Huie and Laszlo,<sup>5</sup> in their kinetic studies, questioned the validity of these spectroscopically derived dissociation energy values. The value from the Durie and Ramsay study is too small to be consistent with the kinetic studies Herron and Huie preferred the results of Phillips and Sugden. Huie and Laszlo adopted an enthalpy of formation based on the molecular beam studies of Radlein *et al.*<sup>6</sup> D<sub>0</sub><sup>°</sup> = 222 ± 13 kJ mol<sup>-1</sup>, and Buss *et al.*<sup>7</sup> D<sub>0</sub><sup>°</sup> = 230 ± 8 kJ mol<sup>-1</sup>. Ruscic and Berkowitz,<sup>8</sup> in determining experimentally the enthalpy of formation and ionization potential of HOBr, inferred a new value for the enthalpy of formation of IO; ΔH<sup>°</sup>(IO, 0 K) = 145 kJ mol<sup>-1</sup>. This value was a mean of the Radlein *et al.*<sup>6</sup> and the spectroscopic results.<sup>12</sup> In concurrence with the arguments of Huie, Herron and Laszlo we adopt D<sub>0</sub><sup>°</sup> = 226 kJ mol<sup>-1</sup> which leads to ΔH<sup>°</sup>(0 K) = 128 ± 18 kJ mol<sup>-1</sup>. Additional data needed for the calculations presented here, e.g. thermal functions for (g), and I<sub>2</sub>(ref), O(g), and O<sub>2</sub>(ref), are taken from JANAF Thermochemical Tables.<sup>9</sup> A recent photoionization study<sup>10</sup> confirms our adopted value.

## Heat Capacity and Entropy

The spectroscopic results tabulated above are for the <sup>171</sup>IO isotope. Isotopic relationships<sup>11</sup> are used to convert the above constants to those natural abundance species. The latter values are then used in the calculation of the thermal functions. Only the X and A states are included in the calculation; a sum-over-states technique is used. Values of ω<sub>e</sub> and ω<sub>e</sub>x<sub>e</sub> are from Bekoooy *et al.*<sup>12</sup> and Gilles *et al.*<sup>13</sup> but the value of D<sub>e</sub> for the excited state is estimated.<sup>11</sup> The dissociation energy of the A state is estimated to be 12900 cm<sup>-1</sup>.

The electronic ground state configuration, X<sup>2</sup>Π<sub>1/2</sub> (inverted doublet) was confirmed by the EPR measurements of Carrington *et al.*<sup>14</sup> An earlier EPR spectra result, 2330 cm<sup>-1</sup>, was reported by Brown *et al.*<sup>15</sup> The recent measured value of Gilles *et al.*<sup>13</sup> 2091 cm<sup>-1</sup>, for the spin-orbit splitting of the ground state is adopted here. For ClO the spin-orbit splitting of the A state was estimated to be 1.5 times the value found for the ground state. Using the same factor of 1.5 the spin-orbit splitting for the A state in IO is estimated to be 3140 cm<sup>-1</sup>. The position of the first excited state, A<sup>1</sup>Π<sub>1/2</sub>, was provided by Bekoooy *et al.*<sup>12</sup> Loeuwenschuss *et al.*<sup>16</sup> and Durie *et al.*<sup>20</sup> We adopt the 21557.81 cm<sup>-1</sup> value of Durie *et al.* Additional excited states have been mentioned by Callear and Metcalf<sup>21</sup> and Saito.<sup>15</sup> The higher states were not included in the thermal function calculations.

## References

1. E. H. Coleman, A. G. Gaydon and W. M. Vaidya, *Nature* **162**, 108–9 (1948).
2. R. A. Durie and D. A. Ramsay, *Can. J. Phys.* **36**, 35–53 (1958).
3. L. F. Phillips and T. M. Sugden, *Trans. Faraday Soc.* **57**, 914–20 (1961).
4. J. H. Herron and R. E. Huie, *J. Phys. Chem.* **73**(5), 1326–35 (1969).
5. R. E. Huie and B. Laszlo, *Adv. Chem. Series*, in press (1995).

Continued on page 1463

Iodine Oxide IO(g)

I<sub>2</sub>O(g)

T/K	C <sub>p</sub> <sup>°</sup> J K <sup>-1</sup> mol <sup>-1</sup>	S <sup>°</sup> J K <sup>-1</sup> mol <sup>-1</sup>	H <sup>°</sup> - H <sup>°</sup> (T) kJ mol <sup>-1</sup>	ΔG <sup>°</sup>	log K <sub>r</sub>
0	.000	INFINITE	-9.003	127.954	INFINITE
50	29.104	186.214	-7.555	123.526	-129.047
100	29.157	206.394	-6.099	117.880	-118.956
150	29.663	218.290	-4.631	117.421	-114.590
200	30.696	226.937	-3.124	126.934	-110.387
250	31.865	233.933	-1.560	126.455	-106.305
298.15	32.900	239.636	.000	126.016	-102.465
300	32.938	239.839	.061	125.999	-102.319
400	34.700	249.567	3.446	117.080	-94.840
500	36.155	257.470	6.991	91.415	-9.550
600	37.433	264.177	10.672	95.221	90.680
700	38.533	270.032	14.472	95.510	89.901
800	39.430	275.239	18.371	95.851	89.075
900	40.121	279.925	22.351	96.233	88.207
1000	40.624	284.180	26.389	96.639	87.292
1100	40.987	288.069	30.470	97.058	86.338
1200	41.184	291.644	34.579	97.476	85.345
1300	41.311	294.946	38.713	97.882	84.317
1400	41.366	298.010	42.839	98.267	83.259
1500	41.371	300.864	46.976	98.619	82.175
1600	41.344	303.533	51.112	98.933	81.069
1700	41.294	306.038	55.244	99.202	79.944
1800	41.229	308.397	59.370	99.419	78.803
1900	41.154	310.624	63.490	99.584	77.654
2000	41.071	312.733	67.601	99.694	76.496
2100	40.980	314.735	71.703	99.749	75.334
2200	40.882	316.639	75.797	99.754	74.172
2300	40.774	318.454	79.879	99.708	73.009
2400	40.655	320.186	83.951	99.618	71.852
2500	40.524	321.844	88.010	99.488	70.695
2600	40.380	323.430	92.056	99.322	69.548
2700	40.221	324.951	96.085	99.123	68.408
2800	40.048	326.411	100.099	98.902	67.272
2900	39.859	327.813	104.095	98.657	66.147
3000	39.656	329.161	108.071	98.392	65.031
3100	39.438	330.458	112.025	98.112	63.922
3200	39.206	331.706	115.958	97.820	62.826
3300	38.966	332.909	119.867	97.517	61.736
3400	38.713	334.068	123.751	97.204	60.659
3500	38.452	335.187	127.609	96.884	59.586
3600	38.184	336.266	131.441	96.558	58.527
3700	37.912	337.309	135.246	96.226	57.473
3800	37.635	338.316	139.023	95.888	56.432
3900	37.358	339.290	142.773	95.546	55.399
4000	37.080	340.233	146.495	95.198	54.371
4100	36.803	341.145	150.189	94.846	53.355
4200	36.529	342.028	153.855	94.489	52.349
4300	36.259	342.885	157.495	94.128	51.348
4400	35.993	343.715	161.107	93.762	50.359
4500	35.734	344.521	164.693	93.390	49.376
4600	35.480	345.304	168.254	93.014	48.401
4700	35.234	346.066	171.790	92.633	47.437
4800	34.996	346.803	175.301	92.246	46.481
4900	34.765	347.523	178.789	91.853	45.528
5000	34.543	348.223	182.254	91.454	44.586
5100	34.328	348.903	185.698	91.050	43.653
5200	34.123	349.569	189.120	90.638	42.730
5300	33.925	350.217	192.523	90.220	41.814
5400	33.736	350.850	195.906	89.795	40.901
5500	33.556	351.467	199.270	89.362	40.001
5600	33.383	352.070	202.617	88.922	39.109
5700	33.218	352.660	205.947	88.474	38.220
5800	33.061	353.236	209.261	88.017	37.344
5900	32.911	353.800	212.559	87.551	36.472
6000	32.768	354.352	215.843	87.076	35.611

PREVIOUS:

CURRENT: March 1996 (1 bar)

Iodine oxide (IO)

$\Delta_f H^\circ(0\text{ K}) = [438 \pm 25] \text{ kJ}\cdot\text{mol}^{-1}$   
 $S^\circ(298.15\text{ K}) = [281.5 \pm 4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

Ideal Gas

$M_r = 158.90327$  Iodine oxide (IO)

$\Delta_f H^\circ(0\text{ K}) = [162.7 \pm 25] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [159.3 \pm 25] \text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum Weight state	$\epsilon_e, \text{cm}^{-1}$	g
$X^2B_1$	0.0	2

Vibrational Frequencies and Degeneracies	
$\nu, \text{cm}^{-1}$	
765(1)	
192(1)	
[800](1)	

Point Group:  $C_{2v}$   
 Bond Distance: I-O = [1.8]Å  
 Bond Angle: O-I-O = [120]°  
 Product of the Moments of Inertia:  $I_A I_B I_C = 725.5989 \times 10^{-117} \text{ g}^3\cdot\text{cm}^6$   
 $\sigma = 2$

Enthalpy of Formation

For the series OXO(g) [where X = F, Cl, Br, I], there are only reliable experimental data for ClO(g).  $\Delta_f H^\circ(\text{ClO})$  and  $\Delta_f H^\circ(\text{IO})$  are reasonable, we adopt the ratio of the numbers (~1.94) to apply for a similar relationship between IO(g) and OIO(g). Thus,  $\Delta_f H^\circ(\text{IO}, 0\text{ K}) = 1.94 \Delta_f H^\circ(\text{ClO}) = 438 \text{ kJ}\cdot\text{mol}^{-1}$ .

Heat Capacity and Entropy

Based on the ESR study by Byberg,<sup>1</sup> the ground state of the free IO<sub>2</sub> molecule belongs to the representation B<sub>1</sub> of the point group C<sub>2v</sub>. This symmetric, bent molecule is estimated to have an O-I-O angle of [120]° and a bond length of [1.8] Å in analogy with the corresponding fluorine, chlorine, and bromine oxide molecules.<sup>2</sup> The principal moments of inertia in g·cm<sup>2</sup> are:  $I_A = 3.4373 \times 10^{-39}$ ,  $I_B = 12.1991 \times 10^{-39}$ , and  $I_C = 16.3491 \times 10^{-39}$ .

Two of the three vibrational frequencies have been derived by Gilles *et al.*,<sup>3</sup> who used photoelectron spectroscopic techniques.  $\nu_3$  is estimated based on anticipated trends with the OXO(g) family<sup>4</sup> and assuming  $\nu_2 > \nu_1$ .

References

- J. R. Byberg, J. Chem. Phys. 88(4), 2129-34 (1988).
- NIST-JANAF Thermochemical Tables: OFO(g): (September 1995); OClO(g): (March 1996); OBrO(g): (March 1996).
- M. K. Gilles, M. L. Polak, and W. C. Lineberger, J. Chem. Phys. 96(11), 8012-20 (1992)

I<sub>2</sub>O<sub>2</sub>(g)

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K			Standard State Pressure = p° = 0.1 MPa			log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (G° - H°(T <sub>r</sub> ))/T	H° - H°(T <sub>r</sub> )	Δ <sub>f</sub> H°	Δ <sub>f</sub> G°	log K <sub>r</sub>	
J·K <sup>-1</sup> ·mol <sup>-1</sup>							
0	.000	INFINITE	INFINITE	162.744	162.744	INFINITE	
50	34.278	211.198	414.979	162.490	160.395	-167.564	
100	37.830	236.126	319.929	161.795	158.563	-82.825	
150	40.093	251.918	294.779	161.091	157.100	-54.707	
200	42.280	263.746	283.600	160.427	155.871	-40.709	
250	44.599	273.429	282.225	159.828	154.803	-32.344	
298.15	46.697	281.468	281.468	159.323	153.882	-26.959	
300	46.772	281.757	281.468	159.304	153.848	-26.787	
400	50.184	295.711	283.348	150.372	152.400	-19.908	
500	52.445	307.170	287.000	148.085	150.097	-16.203	
600	53.929	316.872	291.191	145.408	148.642	-13.966	
700	54.929	325.265	295.473	142.854	148.591	-12.564	
800	55.626	332.648	299.668	140.384	149.253	-11.160	
900	56.127	339.230	303.705	137.973	149.542	-10.221	
1000	56.498	345.164	307.559	135.605	149.811	-9.469	
1100	56.779	350.562	311.226	133.270	150.059	-8.852	
1200	56.997	355.513	314.714	130.959	150.283	-8.336	
1300	57.168	360.082	318.030	128.668	150.480	-7.900	
1400	57.306	364.324	321.187	126.391	150.647	-7.525	
1500	57.419	368.281	324.196	124.128	150.779	-7.200	
1600	57.511	371.990	327.069	121.875	150.870	-6.915	
1700	57.588	375.479	329.815	119.630	150.915	-6.664	
1800	57.653	378.773	332.444	117.392	150.911	-6.440	
1900	57.709	381.893	334.963	115.160	150.855	-6.240	
2000	57.756	384.853	337.386	112.933	150.745	-6.061	
2100	57.797	387.672	339.714	110.711	150.583	-5.898	
2200	57.832	390.361	341.955	108.492	150.374	-5.751	
2300	57.863	392.933	344.116	106.277	150.113	-5.616	
2400	57.891	395.396	346.202	104.065	149.813	-5.493	
2500	57.915	397.760	348.217	101.858	149.476	-5.380	
2600	57.936	400.031	350.167	99.648	149.109	-5.276	
2700	57.955	402.218	352.054	97.432	148.718	-5.181	
2800	57.972	404.326	353.884	95.219	148.309	-5.092	
2900	57.988	406.361	355.659	93.007	147.887	-5.009	
3000	58.002	408.327	357.382	90.796	147.458	-4.933	
3100	58.014	410.229	359.056	88.587	147.026	-4.861	
3200	58.026	412.071	360.684	86.379	146.596	-4.794	
3300	58.036	413.857	362.268	84.172	146.172	-4.732	
3400	58.046	415.590	363.811	81.966	145.756	-4.673	
3500	58.055	417.272	365.315	79.761	145.351	-4.618	
3600	58.063	418.908	366.781	77.557	144.959	-4.566	
3700	58.070	420.499	368.211	75.354	144.581	-4.517	
3800	58.077	422.048	369.608	73.151	144.219	-4.471	
3900	58.083	423.556	370.972	70.948	143.874	-4.427	
4000	58.089	425.027	372.305	68.746	143.546	-4.386	
4100	58.094	426.461	373.608	66.544	143.234	-4.347	
4200	58.099	427.861	374.883	64.342	142.940	-4.309	
4300	58.104	429.228	376.131	62.140	142.663	-4.274	
4400	58.108	430.564	377.353	59.938	142.402	-4.240	
4500	58.112	431.870	378.550	57.736	142.156	-4.208	
4600	58.116	433.147	379.724	55.534	141.926	-4.177	
4700	58.120	434.397	380.874	53.332	141.709	-4.147	
4800	58.123	435.621	382.001	51.130	141.505	-4.119	
4900	58.126	436.819	383.108	48.928	141.313	-4.092	
5000	58.129	437.994	384.194	46.726	141.132	-4.067	
5100	58.132	439.145	385.260	44.524	140.959	-4.042	
5200	58.135	440.274	386.307	42.322	140.795	-4.018	
5300	58.137	441.381	387.336	40.120	140.636	-3.995	
5400	58.140	442.468	388.347	37.918	140.483	-3.973	
5500	58.142	443.535	389.341	35.716	140.333	-3.952	
5600	58.144	444.582	390.318	33.514	140.184	-3.931	
5700	58.146	445.612	391.279	31.312	140.036	-3.912	
5800	58.148	446.623	392.224	29.110	139.886	-3.893	
5900	58.150	447.617	393.155	26.908	139.733	-3.875	
6000	58.151	448.594	394.071	24.706	139.575	-3.857	

PREVIOUS:

CURRENT: March 1996 (1 bar)

Iodine oxide (IO)

I<sub>2</sub>O<sub>2</sub>(g)

Iodine oxide (IOO)

$M_r = 158.90327$

Iodine oxide (IOO)

$I_2O_2(g)$

$\Delta_f H^\circ(0\text{ K}) = [119 \pm 40] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [116.5 \pm 40] \text{ kJ}\cdot\text{mol}^{-1}$

$S^\circ(298.15\text{ K}) = [296.4 \pm 4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

Electronic Level and Quantum state	Weight $g_i$
$X^1A'$	0.0
[2]	

Vibrational Frequencies and Degeneracies

$\nu, \text{cm}^{-1}$
[1500](1)
[150](1)
[275](1)

Point Group  $C_2$   
 Bond Distances: I-O = [2.4]Å; O-O = [1.25]Å  
 Bond Angle I-O-O = [120]°  
 Product of the Moments of Inertia:  $I_A I_B I_C = [1314.2931 \times 10^{-117}] \text{ g}^3\cdot\text{cm}^6$   
 $\sigma = 1$

Enthalpy of Formation

Following trends<sup>1</sup> in the reaction  $XOO(g) \rightarrow X(g) + 2O(g)$ , a reasonable estimate for the iodine reaction would be  $\Delta_f H^\circ(0\text{ K}) = -91.25 \text{ kJ}\cdot\text{mol}^{-1}$ . However, looking at the trends in the reaction  $XOO(g) \rightarrow XO(g) + O(g)$ , a reasonable estimate for the iodine reaction would be  $260 \text{ kJ}\cdot\text{mol}^{-1}$ , which leads to a  $\Delta_f H^\circ(0\text{ K}) = 119 \text{ kJ}\cdot\text{mol}^{-1}$ . This large discrepancy in estimates is a result of the estimates and uncertainties in all XOO enthalpies of formation. We adopt the value based on the reaction involving an X-O bond breakage.

Heat Capacity and Entropy

The vibrational frequencies and structure are estimated based on the existing data for  $FOO(g)$ ,  $ClOO(g)$ , and  $BrOO(g)$ .<sup>1</sup> The principal moments of inertia in  $\text{g}\cdot\text{cm}^2$  are:  $I_A = 1.1391 \times 10^{-39}$ ,  $I_B = 33\,4021 \times 10^{-39}$ , and  $I_C = 34.5412 \times 10^{-39}$ .

References

<sup>1</sup>NIST-JANAF Thermochemical Tables:  $FOO(g)$ ; Sept. 1995,  $ClOO(g)$ ; March 1996;  $BrOO(g)$  (March 1996).

T/K	$C_p^\circ$	$S^\circ - (S^\circ - H^\circ(T))/T$	$H^\circ - H^\circ(T)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log $K_f$
0	.000	INFINITE	-12.806	119.000	119.000	INFINITE
50	35.573	219.838	-11.117	118.762	118.762	-121.430
100	41.565	246.433	-9.181	118.195	118.195	-39.512
150	45.076	264.029	-7.705	117.115	117.115	-11.907
200	46.892	277.272	-6.702	115.797	115.797	-28.738
250	47.962	287.859	-6.035	114.203	114.203	-44.446
298.15	48.727	296.374	-5.547	112.899	112.899	-62.621
300	48.754	296.676	.090	116.523	106.638	-18.682
400	50.151	310.895	5.036	107.664	103.667	-18.557
500	51.463	322.229	10.118	85.389	104.801	-10.948
600	52.620	331.717	15.323	85.758	108.628	-9.457
700	53.581	339.903	20.635	85.951	112.426	-8.389
800	54.355	347.110	26.035	86.103	116.199	-7.587
900	54.973	353.549	31.501	86.270	119.950	-6.962
1000	55.467	359.368	37.024	86.430	123.684	-6.461
1100	55.863	364.674	42.591	86.580	127.402	-6.050
1200	56.184	369.548	48.194	86.718	131.107	-5.707
1300	56.446	374.056	53.826	86.839	134.801	-5.416
1400	56.662	378.288	59.482	86.938	138.487	-5.167
1500	56.842	382.163	65.157	87.009	142.166	-4.951
1600	56.993	385.837	70.849	87.045	145.842	-4.761
1700	57.121	389.296	76.555	87.041	149.517	-4.594
1800	57.230	392.564	82.273	86.997	153.192	-4.446
1900	57.324	395.661	88.001	86.895	156.871	-4.313
2000	57.405	398.603	93.737	86.749	160.559	-4.193
2100	57.475	401.406	99.481	86.554	164.254	-4.086
2200	57.537	404.081	105.232	86.311	167.961	-3.989
2300	57.591	406.640	110.984	86.024	171.678	-3.898
2400	57.639	409.092	116.750	85.698	175.408	-3.818
2500	57.681	411.446	122.516	85.337	179.154	-3.743
2600	57.719	413.709	128.286	84.948	182.914	-3.675
2700	57.753	415.888	134.059	84.536	186.690	-3.612
2800	57.784	417.988	139.836	84.107	190.481	-3.553
2900	57.812	420.017	145.616	83.667	194.288	-3.499
3000	57.836	421.977	151.399	83.220	198.110	-3.449
3100	57.859	423.874	157.177	82.773	201.948	-3.403
3200	57.880	425.711	162.970	82.328	205.798	-3.359
3300	57.899	427.492	168.759	81.889	209.663	-3.319
3400	57.916	429.221	174.550	81.460	213.542	-3.281
3500	57.932	430.900	180.342	81.042	217.433	-3.245
3600	57.946	432.532	186.136	80.638	221.336	-3.211
3700	57.960	434.120	191.932	80.249	225.249	-3.180
3800	57.972	435.666	197.728	79.876	229.174	-3.150
3900	57.983	437.172	203.526	79.521	233.108	-3.122
4000	57.994	438.640	209.325	79.183	237.049	-3.096
4100	58.004	440.072	215.125	78.862	241.000	-3.070
4200	58.013	441.470	220.926	78.559	244.958	-3.047
4300	58.022	442.835	226.727	78.274	248.924	-3.024
4400	58.030	444.169	232.530	78.004	252.895	-3.002
4500	58.037	445.474	238.333	77.751	256.873	-2.982
4600	58.044	446.749	244.137	77.513	260.855	-2.962
4700	58.051	447.998	249.942	77.290	264.844	-2.943
4800	58.057	449.220	255.747	77.079	268.837	-2.926
4900	58.063	450.417	261.553	76.880	272.834	-2.908
5000	58.068	451.590	267.360	76.693	276.835	-2.892
5100	58.073	452.740	273.167	76.514	280.840	-2.876
5200	58.078	453.868	278.974	76.344	284.847	-2.861
5300	58.083	454.974	284.783	76.180	288.859	-2.847
5400	58.087	456.060	290.591	76.021	292.873	-2.833
5500	58.091	457.126	296.400	75.866	296.890	-2.820
5600	58.095	458.172	302.209	75.712	300.911	-2.807
5700	58.099	459.201	308.019	75.559	304.939	-2.794
5800	58.102	460.211	313.829	75.405	308.959	-2.782
5900	58.105	461.204	319.639	75.247	312.986	-2.771
6000	58.109	462.181	325.450	75.085	317.018	-2.760

PREVIOUS:

CURRENT: March 1996 (1 bar)

Iodine oxide (IOO)

$I_2O_2(g)$

Iodine oxide (IO<sub>2</sub>)

Ideal Gas

I<sub>2</sub>O<sub>3</sub> (g)

$S^{\circ}(298.15\text{ K}) = [293.0 \pm 4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

$\Delta_f H^{\circ}(0\text{ K}) = [248 \pm 50] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^{\circ}(298.15\text{ K}) = [241.9 \pm 50] \text{ kJ}\cdot\text{mol}^{-1}$

$M_r = 174.90267$

Electronic Level and Quantum state	Weight $g_i$
[ <sup>1</sup> A <sub>1</sub> ]	0
Vibrational Frequencies and Degeneracies $\nu_i, \text{cm}^{-1}$	
	[780](1)
	[357](1)
	[809](2)
	[326](2)

Point Group: C<sub>2v</sub>  
 Bond Distance: I-O = [1.79]Å  
 Bond Angle: O-I-O = [89]<sup>o</sup>  
 Product of the Moments of Inertia:  $I_A I_B I_C = 3642.3539 \times 10^{-117} \text{ g}^3\cdot\text{cm}^6$   
 $\sigma = 3$

Enthalpy of Formation

We adopt an enthalpy of formation value which is based on an assumed relationship of  $\Delta_f H^{\circ}(\text{IO}_2, \text{g})/3 = 0.9D_f^{\circ}(\text{IO})$ . An enthalpy of formation value has been reported by Farkas and Klein.<sup>1</sup> This value,  $-28 \text{ kcal}\cdot\text{mol}^{-1}$  ( $-117 \text{ kJ}\cdot\text{mol}^{-1}$ ), is derived from absorption spectra measurements of iodate ions in solutions. There is considerable uncertainty in this value, both in terms of the experimental measurements and the fact that the authors have interchanged IO<sub>2</sub> and IO. This corresponds to an average bond energy of 241.9 kJ·mol<sup>-1</sup>. Since this value is greater than D<sub>0</sub><sup>o</sup>(IO), it is suspect.

Heat Capacity and Entropy

The structure of this molecule is estimated to be pyramidal with a O-I-O angle of [89]<sup>o</sup> and a bond length of 1.79Å, in analogy with the corresponding chlorine and bromine oxide molecules. Venkateswarlu and Sundaram,<sup>2</sup> Venkateswarlu and Rajalakshmi,<sup>3</sup> Rao and Santhamma,<sup>4</sup> Rao,<sup>5</sup> and Thiruganasambandam and Mohan<sup>6</sup> assumed the same structure and bond angle for ClO<sub>2</sub>, BrO<sub>2</sub>, and IO<sub>2</sub>. Using Badger's rule, the authors examined the relationship between the vibrational frequencies and force constants for the three pyramidal molecules - ClO<sub>2</sub>, BrO<sub>2</sub>, and IO<sub>2</sub>. Although these authors refer to early measurements of the vibrational frequencies, the values appear to be in part those of the ion IO<sub>2</sub><sup>-</sup>. Their reported values are adopted here although we treat them as estimated values. The vibrational frequencies are derived from the force constants which describe the other halogen oxide molecules. The principal moments of inertia in g·cm<sup>2</sup> are:  $I_A = 14.7650 \times 10^{-39}$ ,  $I_B = 14.7650 \times 10^{-39}$ , and  $I_C = 16.7280 \times 10^{-39}$ .

References

1. L. Farkas and F. S. Klein, J. Chem. Phys. **16**(9), 886-93 (1948).
2. K. Venkateswarlu and S. Sundaram, Proc. Phys. Soc. (London) **A69**, 180-3 (1956).
3. K. Venkateswarlu and K. V. Rajalakshmi, Indian J. Pure Appl. Phys. **1**, 380-2 (1963).
4. C. G. R. Rao and C. Santhamma, Current Sci. **33**(22), 677-8 (1964).
5. C. G. R. Rao, Sci. Cult. **38**(12), 522 (1972).
6. P. Thiruganasambandam and S. Mohan, Indian J. Phys. **52B**, 173-8 (1978).

T/K	Enthalpy Reference Temperature = T <sub>1</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>t</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - H(T <sub>1</sub> )]/T	H <sup>o</sup> - H(T <sub>1</sub> )	Δ <sub>f</sub> H <sup>o</sup>	
0	0	INFINITE	INFINITE	248.000	INFINITE
50	33.412	215.531	-13.505	248.000	248.530
100	38.019	239.747	-11.841	247.013	259.637
150	45.140	256.517	-10.081	245.542	250.613
200	51.557	270.403	-8.001	244.239	253.441
250	57.096	282.519	-5.580	243.210	256.671
298.15	61.560	292.970	-2.860	242.430	260.131
300	61.714	293.351	.114	242.881	263.593
400	68.430	312.098	6.647	233.120	271.416
500	72.681	327.860	13.718	211.505	283.075
600	75.418	341.371	21.133	212.303	297.316
700	77.245	353.143	28.772	213.176	311.416
800	78.511	363.545	36.565	214.073	325.389
900	79.417	372.847	44.462	214.968	339.249
1000	80.086	381.251	52.459	215.851	353.011
1100	80.592	388.909	60.474	216.715	366.685
1200	80.984	395.939	68.553	217.555	380.282
1300	81.293	402.434	76.668	218.367	393.809
1400	81.541	408.467	84.810	219.145	407.275
1500	81.742	414.100	92.975	219.884	420.687
1600	81.908	419.381	101.157	220.578	434.051
1700	82.047	424.351	109.355	221.220	447.373
1800	82.163	429.044	117.566	221.806	460.658
1900	82.262	433.489	125.787	222.334	473.919
2000	82.347	437.711	134.018	222.800	487.142
2100	82.420	441.731	142.256	223.207	500.349
2200	82.484	445.566	150.502	223.554	513.539
2300	82.540	449.234	158.753	223.847	526.712
2400	82.589	452.748	167.010	224.089	539.875
2500	82.632	456.120	175.271	224.286	553.028
2600	82.670	459.362	183.536	224.443	566.175
2700	82.704	462.483	191.804	224.568	579.316
2800	82.735	465.491	200.076	224.665	592.454
2900	82.763	468.395	208.351	224.742	605.586
3000	82.788	471.201	216.629	224.802	618.718
3100	82.810	473.916	224.909	224.852	631.849
3200	82.831	476.545	233.197	224.895	644.976
3300	82.849	479.095	241.475	224.936	658.103
3400	82.866	481.568	249.765	224.977	671.239
3500	82.882	483.970	258.048	225.025	684.353
3600	82.896	486.306	266.337	225.074	697.476
3700	82.910	488.577	274.627	225.133	710.597
3800	82.922	490.788	282.919	225.201	723.718
3900	82.933	492.942	291.212	225.280	736.836
4000	82.943	495.042	299.506	225.369	749.951
4100	82.953	497.090	307.800	225.469	763.065
4200	82.962	499.089	316.096	225.580	776.175
4300	82.971	501.042	324.393	225.703	789.284
4400	82.978	502.949	332.690	225.835	802.388
4500	82.986	504.814	340.988	225.978	815.489
4600	82.993	506.638	349.287	226.130	828.587
4700	82.999	508.423	357.587	226.290	841.683
4800	83.005	510.170	365.887	226.456	854.775
4900	83.011	511.882	374.188	226.629	867.864
5000	83.016	513.559	382.489	226.805	880.949
5100	83.021	515.203	390.791	226.984	894.031
5200	83.026	516.815	399.093	227.165	907.107
5300	83.030	518.397	407.396	227.344	920.182
5400	83.034	519.949	415.699	227.521	933.252
5500	83.038	521.472	424.003	227.693	946.319
5600	83.042	522.969	432.307	227.859	959.385
5700	83.046	524.439	440.611	228.016	972.445
5800	83.049	525.883	448.916	228.162	985.505
5900	83.052	527.303	457.221	228.296	998.559
6000	83.055	528.698	465.527	228.414	1011.615

PREVIOUS.

CURRENT March 1996 (1 bar)

Iodine oxide (IO<sub>2</sub>)

I<sub>2</sub>O<sub>3</sub> (g)

Lead Iodide (PbI)

IDEAL GAS

$M_r = 334.1045$

$I_2Pb_2(g)$

$S^\circ(298.15\text{ K}) = 280.094 \pm 0.21\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

$\Delta H_f^\circ(0\text{ K}) = 110.88 \pm 37.7\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta H_f^\circ(298.15\text{ K}) = 107.74 \pm 37.7\text{ kJ}\cdot\text{mol}^{-1}$

Electronic State	Levels and Quantum Weights	$g_i$
$X^1\Pi_{1/2}$	0	2
$2\Pi_{1/2}$	[8300]	2
$A^1\Delta_1$	20528.5	[4]
$B^1\Sigma_2^-$	33488	[2]

$\omega_e = 160.5\text{ cm}^{-1}$   
 $B_e = [0.02861]\text{ cm}^{-1}$   
 $\omega_e x_e = 0.25\text{ cm}^{-1}$   
 $\alpha_e = [0.00066]\text{ cm}^{-1}$   
 $\sigma = 1$   
 $r_e = [2.736]\text{ \AA}$

Enthalpy of Formation

$\Delta H_f^\circ(\text{PbI}, g, 0\text{ K}) = 26.50 \pm 9\text{ kcal}\cdot\text{mol}^{-1}$  is calculated from  $D_0^\circ = 46 \pm 9\text{ kcal}\cdot\text{mol}^{-1}$  with  $\Delta H_f^\circ(\text{Pb}, g) = 46.91 \pm 0.13\text{ kcal}\cdot\text{mol}^{-1}$  and  $\Delta H_f^\circ(I, g, 0\text{ K}) = 25.633\text{ kcal}\cdot\text{mol}^{-1}$ . The dissociation energy is uncertain. Both Rosen<sup>2</sup> and Gaydon<sup>3</sup> referred to the most probable value of  $D_0^\circ = 1.98\text{ eV}$  determined by Wieland and Newburgh<sup>4</sup> from emission and absorption spectra. Interpretation is difficult and Wieland and Newburgh<sup>4,5</sup> have given possible values of 2.84, 1.98, and 1.36 eV with 1.98 eV given as the most probable value. The linear Birge-Sponer extrapolation of the adopted ground state vibrational constants, derived from emission and absorption spectra ( $v, 0$  36)<sup>6</sup> gives a dissociation energy of 3.18 eV. Correction for the ionic character of PbI as suggested by Hildenbrand<sup>6</sup> gives  $D_0^\circ = 2.7\text{ eV}$  (62.3 kcal·mol<sup>-1</sup>). This is in better agreement with the original  $D_0^\circ = 2.84\text{ eV}$  given by Wieland and Newburgh<sup>4</sup> than it is with  $D_0^\circ = 1.98\text{ eV}$  recommended later.<sup>4</sup> An intercomparison of the dissociation energies of lead<sup>7</sup>, mercury<sup>2</sup> and potassium<sup>8</sup> halides suggests a  $D_0^\circ$  value near 45 kcal·mol<sup>-1</sup>. The rounded value  $D_0^\circ = 2.0 \pm 0.4\text{ eV}$  (46 ± 9 kcal·mol<sup>-1</sup>) listed by Gaydon<sup>3</sup> is adopted.  $\Delta H_f^\circ(\text{PbI}, g, 298.15\text{ K}) = 25.75 \pm 9\text{ kcal}\cdot\text{mol}^{-1}$  is calculated from the selected  $\Delta H_f^\circ(\text{PbI}, g, 0\text{ K}) = 26.5 \pm 9\text{ kcal}\cdot\text{mol}^{-1}$ .

Heat Capacity and Entropy

The vibrational constants are taken from the compilation of Rosen.<sup>2</sup> The electronic states and levels are from Rosen<sup>2</sup> except that the <sup>3</sup>I<sub>1/2</sub> state at 8300 cm<sup>-1</sup> is added in analogy to Pb<sup>1</sup> and PbCl<sup>1</sup>. The value of  $r_e = 2.736\text{ \AA}$  is estimated from a comparison of the sums of the ionic radii of the lead halides with the adopted  $r_e$  values for PbF, PbCl, and PbBr.<sup>1</sup>  $B_e$  is calculated from the adopted  $r_e$ . The value for  $\alpha_e$  is estimated assuming a Morse potential function.

References

- <sup>1</sup>JANAF Thermochemical Tables: Pb(g), 3-31-62; I(g), 12-31-61; PbF(g), 12-31-73, PbCl(g), 6-30-73, PbBr(g), 12-31-73, KF(g), 6-30-69; KCl(g), 3-31-66; KBr(g), 3-31-67; KI(g), 6-30-67.
- <sup>2</sup>B. Rosen, Ed., "Spectroscopic Data Relative to Diatomic Molecules," Pergamon Press, New York, (1970).
- <sup>3</sup>A. G. Gaydon, "Spectroscopic Energies and Spectra of Diatomic Molecules," 3rd ed., Chapman and Hall, London, 330 pp. (1968).
- <sup>4</sup>K. Wieland and R. Newburgh, Helv. Phys. Acta 25, 87 (1952).
- <sup>5</sup>K. Wieland and R. Newburgh, Helv. Phys. Acta 22, 590 (1949).
- <sup>6</sup>D. L. Hildenbrand in "Advances in High Temperature Chemistry," Vol. 1, L. Eyring, Ed., Academic Press, New York, pp 193-215, (1967).

T/K	$C_p^\circ$	$S^\circ - (C_p^\circ - H^\circ(T))/T$	$H^\circ - H^\circ(T)$	$\Delta H_f^\circ$	$\Delta G^\circ$	log $K_r$
0	0	INFINITE	0	110.877	110.877	INFINITE
100	34.581	240.551	-10.339	110.700	91.387	-10.546
200	36.646	265.350	-7.215	109.308	76.588	-10.464
250	36.968	273.565	-3.626	108.536	68.497	-10.377
298.15	37.155	280.094	-1.785	108.536	68.497	-10.377
300	37.160	280.323	0	107.707	60.567	-10.662
350	37.288	286.062	0.069	106.809	52.780	-10.546
400	37.380	291.047	1.930	106.809	45.399	-10.464
450	37.451	295.454	3.797	106.809	38.330	-10.377
500	37.508	299.403	5.668	106.809	31.608	-10.286
600	37.601	306.250	7.542	106.809	25.391	-10.195
700	37.676	312.032	9.417	106.809	19.620	-10.104
800	37.742	317.027	11.292	106.809	14.303	-10.013
900	37.803	321.536	13.167	106.809	9.442	-9.922
1000	37.865	325.522	15.042	106.809	5.146	-9.831
1100	37.931	329.134	16.917	106.809	1.415	-9.740
1200	38.004	332.438	18.792	106.809	-2.854	-9.649
1300	38.088	335.483	20.667	106.809	-7.153	-9.558
1400	38.187	338.309	22.542	106.809	-11.452	-9.467
1500	38.301	340.948	24.417	106.809	-15.751	-9.376
1600	38.433	343.424	26.292	106.809	-20.050	-9.285
1700	38.582	345.758	28.167	106.809	-24.349	-9.194
1800	38.747	347.968	30.042	106.809	-28.648	-9.103
1900	38.926	350.069	31.917	106.809	-32.947	-9.012
2000	39.119	352.069	33.792	106.809	-37.246	-8.921
2100	39.322	353.983	35.667	106.809	-41.545	-8.830
2200	39.533	355.817	37.542	106.809	-45.844	-8.739
2300	39.750	357.579	39.417	106.809	-50.143	-8.648
2400	39.972	359.275	41.292	106.809	-54.442	-8.557
2500	40.196	360.911	43.167	106.809	-58.741	-8.466
2600	40.421	362.492	45.042	106.809	-63.040	-8.375
2700	40.645	364.022	46.917	106.809	-67.339	-8.284
2800	40.867	365.504	48.792	106.809	-71.638	-8.193
2900	41.086	366.942	50.667	106.809	-75.937	-8.102
3000	41.303	368.339	52.542	106.809	-80.236	-8.011
3100	41.515	369.696	54.417	106.809	-84.535	-7.920
3200	41.724	371.018	56.292	106.809	-88.834	-7.829
3300	41.928	372.305	58.167	106.809	-93.133	-7.738
3400	42.128	373.560	60.042	106.809	-97.432	-7.647
3500	42.323	374.784	61.917	106.809	-101.731	-7.556
3600	42.514	375.978	63.792	106.809	-106.030	-7.465
3700	42.702	377.146	65.667	106.809	-110.329	-7.374
3800	42.885	378.287	67.542	106.809	-114.628	-7.283
3900	43.064	379.403	69.417	106.809	-118.927	-7.192
4000	43.240	380.496	71.292	106.809	-123.226	-7.101
4100	43.412	381.566	73.167	106.809	-127.525	-7.010
4200	43.580	382.614	75.042	106.809	-131.824	-6.919
4300	43.746	383.641	76.917	106.809	-136.123	-6.828
4400	43.908	384.649	78.792	106.809	-140.422	-6.737
4500	44.068	385.637	80.667	106.809	-144.721	-6.646
4600	44.224	386.608	82.542	106.809	-149.020	-6.555
4700	44.378	387.560	84.417	106.809	-153.319	-6.464
4800	44.529	388.496	86.292	106.809	-157.618	-6.373
4900	44.678	389.416	88.167	106.809	-161.917	-6.282
5000	44.824	390.326	90.042	106.809	-166.216	-6.191
5100	44.967	391.209	91.917	106.809	-170.515	-6.100
5200	45.108	392.084	93.792	106.809	-174.814	-6.009
5300	45.247	392.944	95.667	106.809	-179.113	-5.918
5400	45.383	393.791	97.542	106.809	-183.412	-5.827
5500	45.516	394.625	99.417	106.809	-187.711	-5.736
5600	45.647	395.447	101.292	106.809	-192.010	-5.645
5700	45.776	396.256	103.167	106.809	-196.309	-5.554
5800	45.902	397.053	105.042	106.809	-200.608	-5.463
5900	46.025	397.839	106.917	106.809	-204.907	-5.372
6000	46.147	398.613	108.792	106.809	-209.206	-5.281

PREVIOUS December 1973 (1 atm)

CURRENT December 1973 (1 bar)

Lead Iodide (PbI)

$I_2Pb_2(g)$

IDEAL GAS

Iodosilylidyne (SiI)

$M_r = 154.9900$  Iodosilylidyne (SiI)

$I_2Si_2(g)$

$S^\circ(298.15\text{ K}) = 253.854\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(0\text{ K}) = 313.51 \pm 41.8\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = 313.63 \pm 41.8\text{ kJ}\cdot\text{mol}^{-1}$

State	$\epsilon$ , $\text{cm}^{-1}$	$g$	Electronic Levels and Molecular Constants ( $\sigma = 1$ ) $\omega_e, \text{cm}^{-1}$ $\omega_e x_e, \text{cm}^{-1}$ $B_e, \text{cm}^{-1}$ $\alpha_e, \text{cm}^{-1}$	$r_e, \text{\AA}$	Source		
$X^1\Pi_{1/2}$	0	2	363.2	0.123	[0.001]	2.45	1
$^2\Pi_{1/2}$	650	2	358.5	1.1	[0.001]	2.45	1 <sub>6</sub>
$A^1\Sigma^+_g$	20939.1	4	275.3	0.118	[0.001]	2.50	1
$A^1\Sigma^+_u$	21204.9	2	208.3	0.085	[0.001]	2.95	1
$B^1\Sigma^+$	32380.3	2	471.0	0.9	[0.123]	[2.45]	1
$C^1\Pi$	42710	4	485	[0.123]	[0.001]	[2.45]	6

Enthalpy of Formation

The adopted value is  $\Delta_f H^\circ(298.15\text{ K}) = 75.0 \pm 10\text{ kcal}\cdot\text{mol}^{-1}$ . The value is based on a Birge-Sponer extrapolation of the  $A^1\Sigma^+$  state by Billingsley<sup>1</sup> who obtains a dissociation limit of  $69.76\text{ kcal}\cdot\text{mol}^{-1}$ . Correction for the ionic character of the bond according to Hildenbrand<sup>2</sup> yields  $D_0 = 57.3\text{ kcal}\cdot\text{mol}^{-1}$  which, with auxiliary JANAF data,<sup>3</sup> gives the adopted value. An uncertainty of  $\pm 10\text{ kcal}\cdot\text{mol}^{-1}$  is assigned to  $\Delta_f H^\circ(298.15\text{ K})$  due to the approximate nature of Birge-Sponer extrapolation based on data from the first few vibrational levels only. The adopted value of  $D_0 = 57.3 \pm 8\text{ kcal}\cdot\text{mol}^{-1}$  is in good agreement with  $D_0 = 56.9$  and  $61.8\text{ kcal}\cdot\text{mol}^{-1}$  obtained in a similar manner from the  $A^1\Sigma^+$  state and ground state data, respectively. The value is also in reasonable agreement with  $D_0 = 72.4$  and  $65 \pm 10\text{ kcal}\cdot\text{mol}^{-1}$  obtained by theoretical and empirical procedures, respectively.<sup>4,5</sup> The upper limit for  $D_0 = 4.02\text{ eV}$  ( $92.7\text{ kcal}\cdot\text{mol}^{-1}$ ) is based on the observed predissociation of the  $B^1\Sigma^+$  state.<sup>1</sup> The adopted value of  $D_0$  is also in good agreement with the average (per bond) heat of atomization of  $SiH_4(g)$  of  $58.6\text{ kcal}\cdot\text{mol}^{-1}$ .<sup>3</sup>

Heat Capacity and Entropy

Electronic levels and molecular constants are taken from the studies by Oldershaw and Robinson<sup>6</sup> and Billingsley.<sup>1</sup> Several systems above  $40,000\text{ cm}^{-1}$  have been observed by Oldershaw and Robinson<sup>7</sup> but are not included since their states and degeneracies are not known. They would make only a minor contribution to the thermodynamic properties at  $6000\text{ K}$  and a negligible contribution at lower temperatures. Of more importance is the uncertainty in the value of the ground state spin splitting constant and the energy of the  $A^1\Sigma^+$  state. Billingsley<sup>1</sup> interprets the observed  $A^1-X$  emission spectrum as terminating at the upper level of the split ground state and calculates the ground state splitting of  $646.4\text{ cm}^{-1}$  from the observation of one absorption line. Lakshminarayana and Harnath<sup>8</sup> observe a second emission series  $650.3\text{ cm}^{-1}$  to the red of that observed by Billingsley, and although the ground state splittings are in agreement, this would place the  $A^1$  state approximately  $650\text{ cm}^{-1}$  lower than reported. We favor Billingsley's interpretation while recognizing the need for additional work to resolve this paradox. In addition the  $B^1\Sigma^+$  state observed for the other silicon monohalides<sup>3</sup> is not observed for SiI. Its energy is difficult to predict due to the rapidly dropping energy of this state across the series and the possible misidentification of this state for SiBr. Accordingly, we have assigned an uncertainty of  $\pm 0.1\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  to  $S^\circ(298.15\text{ K})$  to account for this uncertainty. Since no information is available on the rotational constants for the B and C states, the ground state  $B_e = 123\text{ cm}^{-1}$  was used in our calculations. Likewise, values of  $\alpha_e = .001\text{ cm}^{-1}$  are estimated for all states. The ground state is treated as two distinct levels due to the splitting of this state as expressed by the spin coupling constant ( $A = 650\text{ cm}^{-1}$ ). This leads to slightly biased results at low temperature; the stated uncertainty in  $S^\circ(298.15\text{ K})$  should account for this also. All molecular constants have been corrected to reflect the natural abundance of Si.

References

- J. Billingsley, *J. Mol. Spectrosc.* **43**, 128 (1972).
- D. L. Hildenbrand, "Advances in High Temperature Chemistry," Vol. 1, L. Eyring, ed., Academic Press, NY, (1967).
- JANAF Thermochemical Tables, Si(g), 3-31-67, I(g), 6-30-74, SiI(g), 6-30-76, SiF(g), SiCl(g), SiBr(g), 12-31-76.
- S. P. Tandon and K. Tandon, *J. Phys. Chem.* **38**, 460 (1964).
- O. G. Polyachenok, *Russ. J. Phys. Chem.* **40**, 1420 (1966).
- G. A. Oldershaw and K. Robinson, *Trans. Faraday Soc.* **64**, 2256 (1968).
- G. A. Oldershaw and K. Robinson, *J. Mol. Spectrosc.* **44**, 602 (1972).
- A. Lakshminarayana and P. B. V. Harnath, *Proc. Phys. Soc., London (A)*, **71**, 376 (1970).

T/K	$C_p^\circ$	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$		log K <sub>r</sub>
		$S^\circ - (G^\circ - H^\circ(T_r))/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	
0	0	INFINITE	0	313.510	313.510	INFINITE
100	30.446	216.152	-9.936	286.471	286.471	-154.861
200	35.736	238.883	-7.001	278.371	278.371	-72.703
250	37.748	247.087	-3.691	269.420	269.420	-56.292
298.15	39.038	253.854	0	260.868	260.868	-45.703
300	39.076	254.096	0.072	260.540	260.540	-45.364
350	39.850	260.184	2.047	251.730	251.730	-37.569
400	40.238	265.534	4.051	243.264	243.264	-31.767
450	40.381	270.283	6.067	235.658	235.658	-27.554
500	40.380	274.539	8.087	230.077	230.077	-24.036
600	40.179	281.886	12.116	219.650	219.650	-19.122
700	39.952	288.059	16.120	209.268	209.268	-15.616
800	39.652	293.370	20.098	198.940	198.940	-12.989
900	39.442	298.028	24.052	188.669	188.669	-10.950
1000	39.276	302.175	27.987	178.458	178.458	-9.322
1100	39.151	305.912	31.969	168.309	168.309	-7.992
1200	39.057	309.314	35.819	158.220	158.220	-6.887
1300	38.989	312.438	39.721	148.193	148.193	-5.954
1400	38.943	315.325	43.617	138.228	138.228	-5.157
1500	38.913	318.011	47.510	128.324	128.324	-4.469
1600	38.897	320.522	51.400	118.481	118.481	-3.868
1700	38.891	322.880	55.290	108.749	108.749	-3.354
1800	38.895	325.103	59.179	99.123	99.123	-2.972
1900	38.906	327.206	63.069	89.708	89.708	-2.631
2000	38.924	329.202	66.962	80.662	80.662	-2.326
2100	38.948	331.102	70.854	72.050	72.050	-2.051
2200	38.976	332.914	74.750	63.914	63.914	-1.802
2300	39.010	334.647	78.649	56.249	56.249	-1.576
2400	39.049	336.308	82.552	49.117	49.117	-1.370
2500	39.093	337.903	86.459	42.502	42.502	-1.181
2600	39.143	339.438	90.371	36.364	36.364	-1.008
2700	39.199	340.916	94.288	30.664	30.664	-0.848
2800	39.262	342.343	98.211	25.372	25.372	-0.700
2900	39.333	343.722	102.141	20.464	20.464	-0.564
3000	39.412	345.056	106.078	15.907	15.907	-0.437
3100	39.500	346.350	110.024	11.688	11.688	-0.318
3200	39.598	347.606	113.978	7.737	7.737	-0.208
3300	39.708	348.826	117.944	4.028	4.028	-0.105
3400	39.829	350.013	121.920	0.574	0.574	-0.008
3500	39.963	351.169	125.910	-5.542	-5.542	0.083
3600	40.110	352.297	130.210	-11.23	-11.23	0.166
3700	40.271	353.398	134.932	-17.500	-17.500	0.254
3800	40.448	354.475	140.097	-24.244	-24.244	0.354
3900	40.640	355.528	145.712	-31.484	-31.484	0.474
4000	40.848	356.559	151.783	-39.268	-39.268	0.614
4100	41.072	357.571	158.210	-47.654	-47.654	0.774
4200	41.314	358.563	165.098	-56.700	-56.700	0.954
4300	41.572	359.538	172.456	-66.468	-66.468	1.154
4400	41.848	360.497	180.294	-77.000	-77.000	1.374
4500	42.141	361.441	188.626	-88.364	-88.364	1.614
4600	42.452	362.370	197.566	-100.600	-100.600	1.874
4700	42.781	363.287	207.032	-113.764	-113.764	2.154
4800	43.127	364.191	217.074	-127.900	-127.900	2.454
4900	43.491	365.084	227.362	-143.068	-143.068	2.774
5000	43.872	365.967	237.664	-159.320	-159.320	3.114
5100	44.269	366.839	247.901	-176.624	-176.624	3.474
5200	44.683	367.703	258.116	-195.040	-195.040	3.854
5300	45.113	368.558	268.334	-214.624	-214.624	4.254
5400	45.559	369.406	278.504	-235.440	-235.440	4.674
5500	46.020	370.246	288.664	-257.560	-257.560	5.114
5600	46.496	371.079	298.844	-280.960	-280.960	5.574
5700	46.985	371.906	309.074	-305.720	-305.720	6.054
5800	47.488	372.728	319.274	-331.920	-331.920	6.554
5900	48.003	373.544	329.464	-359.640	-359.640	7.074
6000	48.531	374.355	339.654	-388.960	-388.960	7.614

PREVIOUS: December 1976 (1 atm)

CURRENT: December 1976 (1 bar)

Iodosilylidyne (SiI)

$I_2Si_2(g)$

Strontium Iodide (SrI)

IDEAL GAS

Strontium Iodide (SrI)

I,Sr<sub>1</sub>(g)

$\Delta H_f^\circ(0\text{ K}) = -27.61 \pm 83.7 \text{ kJ mol}^{-1}$   
 $\Delta H_f^\circ(298.15\text{ K}) = -30.49 \pm 83.7 \text{ kJ mol}^{-1}$

$S^\circ(298.15\text{ K}) = 272.213 \pm 0.21 \text{ J K}^{-1} \text{ mol}^{-1}$

Electronic State	Quantum Weights	$g_i$
X $^1\Sigma^+$	0	2
A $^1\Pi$	14422.7	2
	14815.9	
B $^3\Sigma^-$	14748.8	2
C $^3\Pi$	22666.1	2
	23223.4	
D $^3\Sigma^-$	28928.3	2

$\omega_e = 173.9 \text{ cm}^{-1}$   
 $B_e = [0.03554] \text{ cm}^{-1}$   
 $\omega_e x_e = 0.42 \text{ cm}^{-1}$   
 $\alpha_e = [0.00011] \text{ cm}^{-1}$   
 $\sigma = 1$   
 $r_e = [3.03] \text{ \AA}$

Enthalpy of Formation

The adopted  $\Delta_f H^\circ(0\text{ K}) = -6.65 \pm 20 \text{ kcal mol}^{-1}$  is obtained from  $D_0^\circ = 71.5 \text{ kcal mol}^{-1}$  calculated from the ratio  $D_0^\circ(\text{SrI})/D_0^\circ(\text{SrI}_2) = 0.46$ . This value for the ratio was found for a series of mono and dihalides<sup>1</sup> and for other alkaline earth halide systems.<sup>2</sup> Other values for  $D_0^\circ$  kcal mol<sup>-1</sup> are 54.6 obtained from a linear Birge-Sponer extrapolation of  $\omega_e$  and  $\omega_e x_e$  data<sup>3</sup> with a correction for the ionic character of the molecule as described by Hildenbrand,<sup>4</sup> 67.3 obtained by Krasnov and Karaseva<sup>5</sup> as a lower bound from a consideration of ionic bonding forces, and 65 obtained by Mims *et al.*<sup>6</sup> as a lower bound from a consideration of energy conservation and measured reaction threshold relative kinetic energy from crossed molecular beam experiments.  $\Delta_f H^\circ(298.15\text{ K}) = -7.29 \pm 20 \text{ kcal mol}^{-1}$  from the adopted  $\Delta_f H^\circ(0\text{ K}) = -6.65 \text{ kcal mol}^{-1}$ .

Heat Capacity and Entropy

The ground state vibrational constants are from the compilation of Rosen.<sup>3</sup> The value of  $r_e = 3.03 \text{ \AA}$  is assumed the same as the bond distance in  $\text{SrI}_2$ .  $B_e$  is calculated from the adopted  $r_e$ .  $\alpha_e$  is calculated assuming a Morse potential function.  
 The electronic levels and their designations are from Ashrafunnisa *et al.*<sup>7,8</sup> and Reddy *et al.*<sup>10</sup> The data are similar to the values in Rosen<sup>9</sup> but are more complete. The  $D^3\Sigma^-$  level is confirmed by Shah *et al.*<sup>11</sup>

References

- G. D. Blue, J. W. Green, T. C. Ehlert and J. L. Margrave, *Nature* **199**, 804 (1963).
- JANAF Thermochemical Tables: all alkaline earth mono- and di-halides.
- B. Rosen, Ed., "Spectroscopic Data Relative to Diatomic Molecules," Pergamon Press, New York, (1970).
- D. L. Hildenbrand in "Advances in High Temperature Chemistry," Vol. 1, L. Eyring, Ed., Academic Press, New York, pp. 193-215, (1967).
- K. S. Krasnov and N. V. Karaseva, *Optics and Spectrosc.* **19**, 14 (1965).
- C. A. Mims, S. Lin, and R. R. Herm, *J. Chem. Phys.* **57**, 3099 (1972).
- P. A. Akishin, V. P. Spiridonov, G. A. Sobolev, and V. A. Naumov, *Zhur. Fiz. Khim.* **31**, 1871 (1957).
- Ashrafunnisa, D. V. K. Rao and P. T. Rao, *J. Phys.* **B 6**, 1503 (1973).
- Ashrafunnisa, D. V. K. Rao and P. T. Rao, *J. Phys.* **B 6**, 2653 (1973).
- B. R. K. Reddy, Y. P. Reddy, and P. T. Rao, *J. Phys.* **B 4**, 574 (1971).
- S. G. Shah, M. M. Patel and A. B. Darji, *J. Phys.* **B 6**, 1344 (1973).

T/K	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T)]/T$	$H^\circ - H^\circ(T)$	$\Delta_f H^\circ$	Standard State Pressure = $p^\circ = 0.1 \text{ MPa}$	$\log K_r$
0	0	INFINITE	-10.287	-27.614	INFINITE	
100	34.228	232.849	-7.189	-27.540	-44.971	
200	36.539	257.493	-3.620	-28.926	-61.887	
250	36.915	265.691	-1.783	-29.705	-70.044	
298.15	37.135	272.213	0	-30.494	-77.736	
300	37.141	272.443	0.069	-30.526	-78.029	
350	37.294	278.181	1.930	-31.423	-85.877	
400	37.403	283.168	3.797	-40.345	-121.86	
450	37.492	287.579	5.670	-41.891	-159.847	
500	37.563	291.533	7.546	-43.522	-204.304	
600	37.679	298.392	11.309	-64.567	-378.264	
700	37.774	304.208	15.081	-120.241	-632.41	
800	37.859	309.257	18.863	-228.773	-835.418	
900	37.936	313.721	22.653	-388.539	-1135.418	
1000	38.010	317.722	26.450	-529.088	-1472.744	
1100	38.082	321.348	30.255	-70.115	-189.590	
1200	38.152	324.664	34.067	-81.166	-255.906	
1300	38.220	327.771	37.885	-83.221	-328.221	
1400	38.289	330.556	41.711	-85.286	-406.038	
1500	38.358	333.200	45.543	-87.363	-489.565	
1600	38.428	335.678	49.382	-89.459	-579.575	
1700	38.502	338.010	53.229	-92.573	-675.633	
1800	38.580	340.212	57.083	-95.708	-777.662	
1900	38.663	342.301	60.945	-98.958	-885.672	
2000	38.755	344.286	64.816	-102.327	-1000.661	
2100	38.857	346.179	68.696	-105.814	-1123.631	
2200	38.970	347.989	72.587	-109.422	-1254.582	
2300	39.097	349.725	76.491	-113.154	-1394.524	
2400	39.238	351.391	80.407	-117.019	-1543.459	
2500	39.395	352.996	84.339	-121.017	-1701.394	
2600	39.570	354.545	88.287	-125.142	-1869.327	
2700	39.762	356.042	92.353	-129.404	-2047.260	
2800	39.972	357.491	96.546	-133.813	-2235.193	
2900	40.200	358.898	100.968	-138.380	-2433.126	
3000	40.447	360.265	105.624	-143.115	-2641.059	
3100	40.711	361.596	108.338	-148.028	-2859.092	
3200	40.992	362.892	112.423	-153.124	-3087.225	
3300	41.289	364.158	116.537	-158.412	-3325.458	
3400	41.601	365.396	120.682	-163.892	-3573.791	
3500	41.928	366.606	124.858	-169.563	-3832.224	
3600	42.267	367.792	129.068	-175.425	-4100.757	
3700	42.618	368.955	133.312	-181.478	-4379.390	
3800	42.980	370.096	137.592	-187.722	-4668.123	
3900	43.350	371.217	141.908	-194.157	-4967.056	
4000	43.727	372.320	146.262	-200.782	-5276.189	
4100	44.110	373.404	150.654	-207.597	-5595.522	
4200	44.498	374.472	155.084	-214.601	-5925.155	
4300	44.888	375.523	159.553	-221.894	-6265.088	
4400	45.280	376.560	164.062	-229.476	-6615.321	
4500	45.673	377.582	168.609	-237.347	-6975.954	
4600	46.064	378.590	173.196	-245.501	-7347.087	
4700	46.454	379.583	177.822	-253.939	-7728.720	
4800	46.840	380.567	182.487	-262.664	-8120.853	
4900	47.221	381.536	187.190	-271.676	-8523.486	
5000	47.598	382.494	191.931	-280.975	-8936.619	
5100	47.967	383.440	196.709	-290.561	-9360.252	
5200	48.330	384.375	201.524	-300.434	-9794.485	
5300	48.688	385.299	206.375	-310.594	-10239.318	
5400	49.030	386.213	211.261	-321.041	-10694.751	
5500	49.367	387.115	216.181	-331.774	-11160.784	
5600	49.693	388.008	221.134	-342.791	-11637.417	
5700	50.010	388.890	226.119	-354.091	-12124.650	
5800	50.316	389.763	231.135	-365.674	-12622.483	
5900	50.611	390.625	236.188	-377.541	-13130.916	
6000	50.894	391.478	241.257	-389.694	-13650.059	

PREVIOUS: June 1974 (1 atm)

CURRENT: June 1974 (1 bar)

Strontium Iodide (SrI)

I,Sr<sub>1</sub>(g)



Titanium Iodide (TiI)

IDEAL GAS

$M_r = 174.7845$  Titanium Iodide (TiI)

I,Ti(g)

$S^\circ(298.15\text{ K}) = 268.827 \pm 8.4\text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(0\text{ K}) = [275.34 \pm 41.8]\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [274.05 \pm 41.8]\text{ kJ}\cdot\text{mol}^{-1}$

Electronic Levels and Quantum Weights	$g_i$
State	
[ $\Sigma$ ]	
0	[4]
[10000]	[4]
[20000]	[4]
[40000]	[4]
[60000]	[4]
[80000]	[4]
[100000]	[4]

$\omega_e = [240]\text{ cm}^{-1}$   
 $B_e = [0.062]\text{ cm}^{-1}$   
 $\sigma = 1$   
 $r_e = [2.8]\text{ \AA}$

Enthalpy of Formation

The enthalpy of formation,  $\Delta_f H^\circ(298.15\text{ K})$ , of TiI(g) is calculated from the dissociation energy,  $D_0^\circ$ , which is estimated as  $73\text{ kcal}\cdot\text{mol}^{-1}$ . This estimate is obtained from the relation  $\Delta_f H^\circ(\text{TiI}_n, 0\text{ K})/4 < D_0^\circ(\text{TiI}) < \Delta_f H^\circ(\text{TiI}_n, 0\text{ K})/3$ , which is valid for the titanium fluorides. The dissociation energy of TiI(g) from which the relation is derived was estimated relative to that of  $\text{TiF}_4(\text{g})$  by Zimbov and Margrave.<sup>1</sup>

Heat Capacity and Entropy

The vibrational frequency,  $\omega_e$ , and the anharmonic vibrational term,  $\omega_e x_e$ , are estimated from those of  $\text{TiCl}(\text{g})$  and comparisons of the mercury and alkali monohalides. The internuclear distance is estimated from Guggenheimer's relation.<sup>2</sup>  $B_e$  is calculated from  $r_e$ . The ground state term and electronic levels are estimated from the ground state multiplet of  $\text{Ti}^+$ .  $\alpha_e$  is estimated from the Morse potential function.

References

1. K. F. Zimbov and J. L. Margrave, J. Phys. Chem. **71**, 2893 (1967).
2. K. M. Guggenheimer, Proc. Phys. Soc. (London) **58**, 456 (1946).
3. C. E. Moore, U. S. Nat. Bur. Stand. Circ. **467**, (1949).

T/K	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$		log K <sub>r</sub>
	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f G^\circ$	
		$\text{J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	$\text{kJ}\cdot\text{mol}^{-1}$	
0	0	INFINITE	-10.138	275.343	INFINITE
100	32.578	230.074	-7.130	276.266	-134.313
200	36.180	233.948	-5.665	278.299	-62.237
250	37.373	262.151	-1.826	279.709	-47.870
298.15	38.459	268.827	0.	274.052	-38.611
300	38.500	269.065	0.071	274.076	-38.315
350	39.542	275.080	2.073	273.284	-31.507
400	40.464	280.421	4.073	264.546	-26.451
450	41.251	285.734	6.067	263.215	-21.222
500	41.902	289.615	8.146	241.830	-19.773
600	42.842	297.345	12.387	241.368	-15.566
700	43.407	303.995	16.702	240.911	-12.567
800	43.728	309.815	21.060	240.455	-10.322
900	43.903	314.976	25.443	239.952	-8.579
1000	44.002	319.607	29.838	239.325	-7.188
1100	44.066	323.804	34.242	238.506	-6.033
1200	44.119	327.641	38.651	237.504	-5.117
1300	44.175	331.174	43.066	236.311	-4.336
1400	44.238	334.450	47.487	234.929	-3.668
1500	44.312	337.505	51.914	233.473	-3.090
1600	44.395	340.367	56.349	231.934	-2.587
1700	44.487	343.062	60.793	229.988	-2.152
1800	44.585	345.607	65.247	228.887	-1.784
1900	44.687	348.020	69.710	227.618	-1.464
2000	44.791	350.315	74.184	226.180	-1.104
2100	44.896	352.503	78.669	224.586	-0.842
2200	45.001	354.594	83.163	222.856	-0.607
2300	45.103	356.597	87.669	220.991	-0.395
2400	45.203	358.518	92.184	218.997	-0.203
2500	45.299	360.366	96.709	216.947	-0.028
2600	45.391	362.144	101.244	214.835	0.131
2700	45.479	363.859	105.787	212.656	0.277
2800	45.562	365.514	110.339	210.406	0.410
2900	45.641	367.115	114.900	208.081	0.533
3000	45.716	368.663	119.468	205.684	0.646
3100	45.787	370.163	124.043	203.218	0.750
3200	45.854	371.618	128.625	200.684	0.847
3300	45.917	373.030	133.213	198.096	0.937
3400	45.977	374.402	137.808	195.457	1.020
3500	46.034	375.735	142.409	192.752	1.098
3600	46.089	377.033	147.015	190.000	1.170
3700	46.141	378.296	151.626	187.212	1.238
3800	46.191	379.528	156.243	184.394	1.309
3900	46.240	380.728	160.864	181.551	1.385
4000	46.287	381.899	165.491	178.689	1.464
4100	46.333	383.043	170.122	175.812	1.546
4200	46.378	384.160	174.757	172.925	1.631
4300	46.422	385.252	179.397	170.021	1.719
4400	46.466	386.319	184.042	167.104	1.809
4500	46.510	387.364	188.691	164.176	1.901
4600	46.554	388.387	193.344	161.235	1.995
4700	46.597	389.388	198.001	158.284	2.091
4800	46.641	390.370	202.663	155.328	2.188
4900	46.686	391.332	207.329	152.361	2.286
5000	46.731	392.276	212.000	149.385	2.385
5100	46.776	393.202	216.676	146.403	2.485
5200	46.823	394.110	221.356	143.418	2.586
5300	46.869	395.003	226.040	140.430	2.688
5400	46.917	395.879	230.730	137.440	2.791
5500	46.966	396.741	235.424	134.448	2.895
5600	47.015	397.587	240.123	131.454	3.000
5700	47.066	398.420	244.827	128.458	3.106
5800	47.117	399.239	249.536	125.461	3.213
5900	47.170	400.045	254.250	122.463	3.321
6000	47.223	400.838	258.970	119.464	3.430

PREVIOUS: December 1968 (a atm)

CURRENT: December 1968 (1 bar)

Titanium Iodide (TiI)

I,Ti(g)

Zirconium Iodide (ZrI)

IDEAL GAS

$M_r = 218.1245$  Zirconium Iodide (ZrI)

$I_2ZrI_2(g)$

$S^\circ(298.15\text{ K}) = [275.805] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(0\text{ K}) = [593.20 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [591.20 \pm 41.8] \text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum State	Weight $g_i$
$\sum$	4

$\omega_e x_e = [223] \text{ cm}^{-1}$   
 $B_e = [0.03789] \text{ cm}^{-1}$   
 $\omega_e x_e = [1.2] \text{ cm}^{-1}$   
 $\alpha_e = [0.00020] \text{ cm}^{-1}$   
 $\sigma = 1$   
 $r_e = [2.9] \text{ \AA}$

Enthalpy of Formation

The dissociation energy was estimated from a correlation of the JANAF values for  $TiCl(g)$ ,  $TiI(g)$ , and  $ZrCl(g)$ . The resulting value, 29.7 kcal·mol<sup>-1</sup>, was employed with auxiliary JANAF enthalpies of formation for  $Zr(g)$  and  $I(g)$  in calculating  $\Delta_f H^\circ(298.15\text{ K})$ .

Heat Capacity and Entropy

The vibrational frequency was estimated from those of  $TiI(g)$ ,  $TiCl(g)$ , and the alkali halides. The ground state configuration was assumed to be analogous to the ground term of  $TiCl(g)$  as given by Shenyavskaya *et al.*<sup>1</sup> The internuclear distance was estimated from those of  $TiBr(g)$ ,  $TiI(g)$  and  $ZrI_4(g)$ .

Reference

<sup>1</sup>E. A. Shenyavskaya *et al.*, *Optics and Spectroscopy* **12**, 359 (1962).

T/K	$C_p^\circ$	$S^\circ$	$S^\circ - (G^\circ - H^\circ(T))/T$	$H^\circ - H^\circ(T)$	$\Delta_f H^\circ$	Standard State Pressure = $p^\circ = 0.1\text{ MPa}$	$\log K_r$
0	0	0	INFINITE	INFINITE	INFINITE	INFINITE	INFINITE
100	36.964	237.198	379.908	-10.097	593.198	593.198	-9.359
200	36.028	261.223	379.160	-7.071	593.813	594.549	-9.011
250	36.593	269.329	378.411	-3.587	592.637	565.699	-8.134
298.15	36.931	275.805	378.805	0	591.925	546.345	-7.194
300	36.941	276.033	378.806	0.068	591.171	537.871	-6.923
350	37.177	281.747	377.256	1.922	590.347	531.540	-6.759
400	37.349	286.723	377.260	3.785	589.508	528.899	-6.799
450	37.483	291.130	378.019	5.656	588.058	520.185	-6.902
500	37.592	295.083	380.019	7.533	585.533	507.090	-7.275
600	37.767	301.955	383.120	11.301	587.733	496.875	-8.257
700	37.910	307.788	386.237	15.085	586.867	486.600	-9.325
800	38.014	311.838	389.255	18.862	585.925	476.353	-10.473
900	38.148	315.345	392.132	22.692	584.892	467.031	-11.708
1000	38.236	318.370	394.838	26.512	583.755	457.528	-13.068
1100	38.360	325.021	399.436	30.343	582.507	447.745	-14.556
1200	38.460	328.363	399.876	34.184	581.150	437.502	-16.168
1300	38.539	331.445	302.188	38.035	546.484	429.463	-17.925
1400	38.636	334.306	304.381	41.895	545.491	420.498	-19.829
1500	38.751	336.976	306.466	45.766	544.434	411.607	-21.873
1600	38.847	339.480	308.452	49.646	543.298	402.788	-24.067
1700	38.941	341.838	310.347	53.534	542.069	394.043	-26.411
1800	39.035	344.067	312.159	57.435	540.732	385.374	-28.905
1900	39.128	346.180	313.894	61.342	539.274	376.782	-31.549
2000	39.221	348.189	315.559	65.260	537.685	368.270	-34.343
2100	39.314	350.105	317.159	69.186	535.954	359.842	-37.287
2200	39.407	351.936	318.699	73.122	534.083	352.244	-40.391
2300	39.499	353.690	320.182	77.068	532.070	345.003	-43.655
2400	39.592	355.373	321.613	81.022	530.906	337.869	-47.089
2500	39.684	356.991	322.996	84.986	505.364	330.838	-50.693
2600	39.776	358.549	324.334	88.959	502.889	323.906	-54.467
2700	39.868	360.052	325.629	92.941	500.419	317.069	-58.411
2800	39.960	361.503	326.885	96.933	497.959	310.323	-62.525
2900	40.052	362.907	328.103	100.933	495.513	303.665	-66.809
3000	40.143	364.267	329.286	104.943	493.087	297.091	-71.263
3100	40.235	365.584	330.435	108.962	490.685	290.598	-75.887
3200	40.327	366.863	331.554	112.990	488.311	284.181	-80.681
3300	40.418	368.106	332.643	117.027	485.968	277.838	-85.645
3400	40.510	369.314	333.704	121.074	483.658	271.566	-90.779
3500	40.602	370.489	334.738	125.129	481.383	265.361	-96.083
3600	40.693	371.634	335.747	129.194	479.145	259.221	-101.657
3700	40.785	372.751	336.732	133.268	476.945	253.142	-107.401
3800	40.876	373.839	337.694	137.351	474.783	247.123	-113.315
3900	40.968	374.902	338.635	141.443	472.660	241.159	-119.399
4000	41.059	375.941	339.555	145.544	470.576	235.250	-125.753
4100	41.150	376.956	340.454	149.655	468.531	229.392	-132.377
4200	41.242	377.948	341.335	153.774	466.524	223.584	-139.281
4300	41.333	378.920	342.198	157.903	464.555	217.823	-146.465
4400	41.425	379.871	343.044	162.041	462.623	212.107	-153.939
4500	41.516	380.803	343.872	166.188	460.728	206.435	-161.703
4600	41.607	381.717	344.685	170.344	458.868	200.805	-169.767
4700	41.699	382.612	345.483	174.510	457.043	195.215	-178.131
4800	41.790	383.491	346.265	178.684	455.254	189.660	-186.805
4900	41.881	384.354	347.034	182.868	453.500	184.141	-195.789
5000	41.973	385.201	347.789	187.060	451.782	178.650	-205.093
5100	42.064	386.033	348.531	191.262	450.100	173.188	-214.727
5200	42.155	386.851	349.260	195.473	448.454	167.754	-224.691
5300	42.247	387.655	349.977	199.693	446.843	162.347	-234.985
5400	42.338	388.445	350.682	203.923	445.266	156.966	-245.609
5500	42.429	389.223	351.375	208.161	443.722	151.618	-256.563
5600	42.521	389.988	352.058	212.408	442.210	146.299	-267.847
5700	42.612	390.742	352.730	216.665	440.728	141.010	-279.461
5800	42.703	391.483	353.392	220.931	439.276	135.751	-291.405
5900	42.795	392.214	354.044	225.206	437.854	130.522	-303.679
6000	42.886	392.934	354.686	229.490	436.462	125.324	-316.283

PREVIOUS September 1964 (1 atm)

CURRENT September 1964 (1 bar)

Zirconium Iodide (ZrI)

$I_2ZrI_2(g)$

Iodine (I<sub>2</sub>)

M<sub>r</sub> = 253.8090 Iodine (I<sub>2</sub>)

REFERENCE STATE

0 to 386.75 K crystal  
386.75 to 457.666 K liquid  
above 457.666 K diatomic ideal gas

Refer to the individual tables for details.

I<sub>2</sub>(ref)

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	Δ <sub>r</sub> H°	
	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·K <sup>-1</sup> ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	
0	0	INFINITE	-13.198	0	0
100	45.650	60.992	-10.148	0	0
200	51.566	94.958	-5.216	0	0
298.15	54.436	116.142	0	0	0
300	54.506	116.479	0.101	0	0
386.750	63.545	131.224	5.153	CRYSTAL <--> LIQUID	
386.750	80.669	171.344	20.670	TRANSITION	
400	80.669	174.062	21.739	0	0
457.666	80.669	184.976	26.391	LIQUID <--> IDEAL GAS	
457.666	37.386	276.609	68.351	FUGACITY = 1 bar	
500	37.464	279.920	69.935	0	0
600	37.612	286.764	73.690	0	0
700	37.735	292.571	77.457	0	0
800	37.847	297.618	81.236	0	0
900	37.959	302.082	85.027	0	0
1000	38.081	306.087	88.828	0	0
1100	38.232	309.724	92.644	0	0
1200	38.431	313.058	96.476	0	0
1300	38.699	316.144	100.332	0	0
1400	39.055	319.025	104.219	0	0
1500	39.507	321.734	108.146	0	0
1600	40.051	324.301	112.124	0	0
1700	40.674	326.747	116.159	0	0
1800	41.352	329.091	120.260	0	0
1900	42.054	331.346	124.431	0	0
2000	42.748	333.521	128.671	0	0
2100	43.404	335.622	132.979	0	0
2200	43.994	337.655	137.349	0	0
2300	44.494	339.622	141.775	0	0
2400	44.890	341.525	146.245	0	0
2500	45.171	343.363	150.749	0	0
2600	45.335	345.139	155.275	0	0
2700	45.382	346.851	159.812	0	0
2800	45.319	348.500	164.348	0	0
2900	45.154	350.088	168.872	0	0
3000	44.897	351.615	173.376	0	0
3100	44.561	353.082	177.849	0	0
3200	44.157	354.490	182.286	0	0
3300	43.697	355.842	186.679	0	0
3400	43.193	357.139	191.024	0	0
3500	42.654	358.384	195.316	0	0
3600	42.091	359.577	199.554	0	0
3700	41.510	360.723	203.734	0	0
3800	40.919	361.822	207.855	0	0
3900	40.325	362.877	211.917	0	0
4000	39.731	363.891	215.920	0	0
4100	39.143	364.864	219.864	0	0
4200	38.563	365.801	223.749	0	0
4300	37.995	366.701	227.577	0	0
4400	37.439	367.568	231.348	0	0
4500	36.899	368.404	235.065	0	0
4600	36.374	369.209	238.729	0	0
4700	35.866	369.986	242.341	0	0
4800	35.375	370.736	245.903	0	0
4900	34.901	371.460	249.416	0	0
5000	34.444	372.161	252.883	0	0
5100	34.005	372.838	256.306	0	0
5200	33.582	373.495	259.685	0	0
5300	33.176	374.130	263.023	0	0
5400	32.785	374.747	266.321	0	0
5500	32.410	375.345	269.580	0	0
5600	32.051	375.926	272.803	0	0
5700	31.705	376.490	275.991	0	0
5800	31.374	377.038	279.145	0	0
5900	31.056	377.572	282.266	0	0
6000	30.751	378.091	285.356	0	0

PREVIOUS: September 1961 (1 atm)

CURRENT: June 1982 (1 bar)

Iodine (I<sub>2</sub>)

I<sub>2</sub>(ref)

I<sub>2</sub>(cr)Iodine (I<sub>2</sub>)

CRYSTAL

Iodine (I<sub>2</sub>)M<sub>r</sub> = 253.8090

$$\Delta_f H^\circ(0 \text{ K}) = 0 \text{ kJ mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = 0 \text{ kJ mol}^{-1}$$

$$\Delta_{\text{fus}} H^\circ = 15.517 \pm 0.16 \text{ kJ mol}^{-1}$$

$$S^\circ(298.15 \text{ K}) = 116.142 \pm 0.080 \text{ J K}^{-1} \text{ mol}^{-1}$$

$$T_{\text{fus}} = 386.75 \pm 0.3 \text{ K}$$

**Enthalpy of Formation**

Zero by definition.

**Heat Capacity and Entropy**

The heat capacity measurements of Shirley and Giauque<sup>1</sup> over the temperature range 13 to 327 K are adopted. No weight is given to the earlier work of Lange<sup>2</sup> which deviate by 1% or more. Carpenter and Harle<sup>3</sup> measured the heat capacity of crystalline and liquid iodine by an adiabatic method. Their data are in poor agreement with Shirley and Giauque<sup>1</sup> in the range 275–330 K and are given no weight. Frederick and Hildebrand<sup>4</sup> measured the enthalpy of crystalline and liquid iodine relative to 298.15 K by the method of mixtures. For calibration they used a slug of copper. The enthalpy of copper which they used appears to be too high. The results are corrected by a factor which varies from 0 at 300 K to 0.995 at 400 K, and 0.990 at 500 K. Using these corrected enthalpies and the heat capacities of Shirley and Giauque<sup>1</sup> above 298.15 K, the following equation is derived for I<sub>2</sub>(cr).  $H^\circ(T) - H^\circ(298.15 \text{ K}) = -50.646T + 0.12345T^2 - 27.97 \times 10^3 T^{-1} + 13508.7$ .

The CODATA recommendation<sup>6</sup> for  $S^\circ(298.15 \text{ K})$  is within 0.003 J K<sup>-1</sup> mol<sup>-1</sup> of our calculated value and is based on the same heat capacity study.<sup>1</sup>

**Fusion Data**

$T_{\text{fus}} = 113.6^\circ \text{C}$  is given by Frederick and Hildebrand.<sup>4</sup> The difference in the enthalpy equations at  $T_{\text{fus}}$  is the enthalpy of fusion.

**Sublimation Data**

Refer to the I<sub>2</sub>(g) table for details.

**References**

- <sup>1</sup>D. A. Shirley and W. F. Giauque, *J. Am. Chem. Soc.* **81**, 4778 (1959).
- <sup>2</sup>E. Lange, *Z. physik. Chem.* **110**, 343 (1924).
- <sup>3</sup>L. G. Carpenter and T. F. Harle, *Phil. Mag.* **23**, 193 (1937).
- <sup>4</sup>K. J. Frederick and J. H. Hildebrand, *J. Am. Chem. Soc.* **60**, 1436 (1939).
- <sup>5</sup>JANAF Thermochemical Tables: Cu(cr), 6–30–77.
- <sup>6</sup>J. D. Cox, Chairman, CODATA Task Group on Key Values for Chemical Thermodynamics, *J. Chem. Thermodyn.* **10**, 903 (1978).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>a</sup>	S <sup>b</sup> - [(C <sub>p</sub> - H <sup>c</sup> (T))/T]	H <sup>c</sup> - H <sup>c</sup> (T <sub>r</sub> )	Δ <sub>r</sub> H <sup>c</sup>	
0	0	0	0	0	0
100	45.650	INFINITE	-13.198	0	0
200	31.566	162.472	-10.148	0	0
250	35.244	94.958	-5.216	0	0
		106.678	-2.588	0	0
298.15	54.436	116.142	0	0	0
300	54.506	116.479	0.101	0	0
350	58.605	125.140	2.913	0	0
386.750	63.545	131.224	5.153	---	---
		117.899	CRYSTAL <--> LIQUID		
400	65.598	133.398	6.009	-15.730	-0.070
450	73.402	141.575	9.484	-16.288	-0.303
500	81.207	149.713	13.349	-16.586	-0.890
600	96.816	165.898	22.250	-51.439	-1.835
700	112.425	181.993	32.712	-44.745	-2.437

PREVIOUS

CURRENT: June 1982

Iodine (I<sub>2</sub>)I<sub>2</sub>(cr)

I<sub>2</sub>(l)

Iodine (I<sub>2</sub>)

LIQUID

Iodine (I<sub>2</sub>)

$S^{\circ}(298.15\text{ K}) = [150.356] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = 386.75 \pm 0.03 \text{ K}$

$\Delta H^{\circ}(298.15\text{ K}) = [13.523] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{liq}}H^{\circ} = 15.517 \pm 0.16 \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**

$\Delta H_f^{\circ}(\text{I}_2, \text{l}, 298.15\text{ K})$  is calculated from that of the crystal by adding  $\Delta_{\text{liq}}H^{\circ}$  and the difference in enthalpy,  $H^{\circ}(386.75\text{ K}) - H^{\circ}(298.15\text{ K})$ , between the crystal and liquid.

**Heat Capacity and Entropy**

The heat capacity of the liquid is adopted to be a constant value,  $80.672 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ , based on the data of Frederick and Hildebrand.<sup>1</sup> Their enthalpy data was corrected as discussed in the I<sub>2</sub>(cr) table. The enthalpy equation is  $H^{\circ}(T) - H^{\circ}(298.15\text{ K}) = 80.672 T - 10529$ . The entropy is calculated in a manner analogous to that used for the enthalpy of formation.

**Vaporization Data**

Refer to the I<sub>2</sub>(g) table for details.

**References**

<sup>1</sup>K. J. Frederick and J. H. Hildebrand, *J. Am. Chem. Soc.* **60**, 1436 (1938).

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa	
		S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>liq</sub> H <sup>o</sup>	Δ <sub>cr</sub> G <sup>o</sup>
0					
100					
200					
250					
298.15	80.669	150.356	0.	13.523	3.322
300	80.669	150.855	0.149	13.571	3.259
350	80.669	163.290	4.183	14.793	1.440
386.750	80.669	171.344	7.147	---	---
400	80.669	174.062	8.216	0.	0.
450	80.669	183.563	12.250	0.	0.
457.666	80.669	184.926	12.868	---	---
500	80.669	192.062	16.283	-40.130	3.799
600	80.669	206.770	24.350	-35.817	12.179
700	80.669	219.205	32.417	-31.518	19.839
800	80.669	229.977	40.484	-27.230	26.883
900	80.669	239.478	48.550	-22.953	33.390
1000	80.669	247.978	56.617	-18.688	39.421

CRYSTAL <-- LIQUID

FUGACITY = 1 bar

PREVIOUS: September 1961

CURRENT: June 1982

Iodine (I<sub>2</sub>)

I<sub>2</sub>(l)

CRYSTAL-LIQUID

0 to 386.75 K crystal  
above 386.75 K liquid

Refer to the individual tables for details.

Iodine (I<sub>2</sub>)

M<sub>r</sub> = 253.8090 Iodine (I<sub>2</sub>)

I<sub>2</sub>(cr,l)

T/K	C <sub>p</sub> <sup>a</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
		S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	Δ <sub>l</sub> H°	Δ <sub>l</sub> G°	
0	0	INFINITE	-13.198	0	0	0
100	45.650	60.992	-10.148	0	0	0
200	51.566	94.958	-5.216	0	0	0
250	53.244	106.678	-2.588	0	0	0
298.15	54.436	116.142	0	0	0	0
300	54.506	116.479	0.101	0	0	0
350	58.605	125.140	2.913	0	0	0
386.750	63.545	131.224	5.153	0	0	0
386.750	80.669	171.344	20.670	CRYSTAL <---> LIQUID TRANSITION	0	0
400	80.669	174.062	21.739	0	0	0
450	80.669	183.563	25.772	0	0	0
457.666	80.669	184.926	26.391	--- FUGACITY = 1 bar ---	0	0
500	80.669	192.062	29.806	-40.130	3.799	-0.397
600	80.669	206.770	37.873	-35.817	12.179	-1.060
700	80.669	219.205	45.940	-31.518	19.839	-1.480
800	80.669	229.977	54.006	-27.250	26.883	-1.755
900	80.669	239.478	62.073	-22.953	33.390	-1.938
1000	80.669	247.978	70.140	-18.688	39.421	-2.059

PREVIOUS.

CURRENT. June 1982

Iodine (I<sub>2</sub>)

I<sub>2</sub>(cr,l)

Iodine (I<sub>2</sub>)

IDEAL GAS

Iodine (I<sub>2</sub>)

I<sub>2</sub>(g)

D<sub>0</sub><sup>o</sup> = 148.816 ± 0.001 kJ·mol<sup>-1</sup>  
 S<sup>o</sup>(298.15 K) = 260.685 ± 0.062 J·K<sup>-1</sup>·mol<sup>-1</sup>

ΔH<sup>o</sup>(0 K) = 65.504 ± 0.092 kJ·mol<sup>-1</sup>  
 ΔH<sup>o</sup>(298.15 K) = 62.421 ± 0.079 kJ·mol<sup>-1</sup>

M<sub>r</sub> = 253.8090

State	T <sub>c</sub>	D <sup>o</sup>	ω <sub>e</sub>	ω <sub>e</sub> x <sub>e</sub>	B <sub>e</sub>	10 <sup>3</sup> α <sub>e</sub>	10 <sup>6</sup> D <sub>e</sub>	r <sub>e</sub> , Å	References
Σ <sub>g</sub> <sup>+</sup>	0	12440	214.5481	0.616259(a)	0.037395	0.12435(b)	0.00454(c)	2.6657	1, 4, 6
<sup>3</sup> Π <sub>u</sub>	10200	12440	110.366	1.3927 <sup>d</sup>	0.028	0.1	0.04	3.104	2
<sup>1</sup> Π <sub>u</sub>	11059	12440	90.6	2.57 <sup>e</sup>	0.02763	0.542 <sup>f</sup>	0.03	3.101	3
<sup>3</sup> Π <sub>g</sub>	15769.01	20043.15	125.697	0.029039	0.1582 <sup>h</sup>	0.00543 <sup>i</sup>		3.0247	4
				(a) +7.507 × 10 <sup>-5</sup> (v+1/2) <sup>3</sup> + 1.263643 × 10 <sup>-6</sup> (v+1/2) <sup>4</sup> + 6.198129 × 10 <sup>-6</sup> (v+1/2) <sup>5</sup> - 2.0255975 × 10 <sup>-7</sup> (v+1/2) <sup>6</sup> + 3.9662824 × 10 <sup>-7</sup> (v+1/2) <sup>7</sup> (b) +4.498 × 10 <sup>-11</sup> (v+1/2) <sup>2</sup> - 1.482 × 10 <sup>-9</sup> (v+1/2) <sup>3</sup> (c) +1.7 × 10 <sup>-11</sup> (v+1/2) + 7 × 10 <sup>-12</sup> (v+1/2) <sup>2</sup> (d) -3.45 × 10 <sup>-2</sup> (v+1/2) <sup>3</sup> (e) +3.36 × 10 <sup>-2</sup> (v+1/2) <sup>3</sup> (f) +2.46 × 10 <sup>-6</sup> (v+1/2) <sup>2</sup> (g) -1.78 × 10 <sup>-3</sup> (v+1/2) <sup>3</sup> + 1.03 × 10 <sup>-6</sup> (v+1/2) <sup>4</sup> (h) -3.36 × 10 <sup>-7</sup> (v+1/2) <sup>2</sup> - 4.78 × 10 <sup>-7</sup> (v+1/2) <sup>3</sup> (i) +3.0 × 10 <sup>-10</sup> (v+1/2)					

The dissociation energy of each state is relative to the lowest level of the ground state; the <sup>3</sup>Π<sub>g</sub><sup>o</sup> state dissociates to I(<sup>2</sup>P<sub>1/2</sub>) + I(<sup>2</sup>P<sub>3/2</sub>).

Enthalpy of Formation

We adopt the enthalpy of formation values of CODATA<sup>5</sup> as follows: ΔH<sup>o</sup>(298.15 K) = 62.421 ± 0.079 kJ·mol<sup>-1</sup> and ΔH<sup>o</sup>(0 K) = 65.500 ± 0.092 kJ·mol<sup>-1</sup>. These values are based on the heat capacity study of Shirley and Gianque<sup>8</sup> and the vapor pressure data of Baxter *et al.*,<sup>9</sup> Baxter and Grosse,<sup>10</sup> Gillespie and Fraser,<sup>11</sup> and Stern.<sup>12</sup> Note that the latter value of ΔH<sup>o</sup> is deduced from the former using the CODATA values of H<sup>o</sup>(298.15 K) for I(g) and I<sub>2</sub>(g). Our calculated value of H<sup>o</sup>(298.15 K) for I<sub>2</sub>(g) is only 1.5 J·mol<sup>-1</sup> smaller than that recommended by CODATA. We adopted the dissociation energy for the Σ<sub>g</sub><sup>+</sup>, <sup>3</sup>Π<sub>u</sub>, and <sup>1</sup>Π<sub>u</sub> states as given by Huber *et al.*<sup>4</sup> The D<sub>0</sub> value for the <sup>3</sup>Π<sub>g</sub> state was deduced from the dissociative state energies given by Gurvich *et al.*<sup>7</sup> (table 10.1). Refer to the monatomic iodine gas table for additional discussion of the dissociation energy.

Heat Capacity and Entropy

The thermal functions are calculated using a direct summation technique. Included in the calculation are the ground state and the three lowest lying excited electronic states. Spectroscopic constants for the ground state are from Leroy;<sup>1</sup> however, we truncate the B<sub>e</sub> expression and of Huber and Herzberg<sup>1</sup> for the <sup>3</sup>Π<sub>u</sub> state. For the ground state and the <sup>3</sup>Π<sub>u</sub> state, the calculation is performed including the quasi-bound rotational levels above the dissociation limit (see Cl<sub>2</sub>(g) table). The values of J<sub>lim</sub> and v<sub>max</sub> for the ground state are those given by Gurvich *et al.*<sup>2</sup> The corresponding values for the <sup>3</sup>Π<sub>u</sub> state were estimated as J<sub>lim</sub> = 500 and v<sub>max</sub> = 69 based on the spectroscopic constants given by Gurvich *et al.*<sup>2</sup> and Ashby.<sup>3</sup>

Splitting of the rotational levels due to the rotational-electronic interaction is taken into account only insofar as the statistical weight of the rotational levels is increased appropriately. The rotational levels are extrapolated to high J values according to the method of Khachikurov<sup>6</sup> who proposed a simpler form of Woolley's method.<sup>7</sup> Our calculated value of S<sup>o</sup>(298.15 K) is only 0.112 J·K<sup>-1</sup>·mol<sup>-1</sup> larger than that given by Gurvich<sup>2</sup> and CODATA.<sup>5</sup>

References

- R. J. Leroy, *J. Chem. Phys.* **52**, 2683 (1970).
- L. V. Gurvich, I. V. Veits and V. A. Medvedev, "Thermodynamic Properties of Individual Substances," Nauka, Moscow, USSR (1978) Vol. 1, Table 10.3. Nauka, Moscow, (1978).
- R. A. Ashby, *Can. J. Phys.* **57**, 698 (1979).
- K. P. Huber and G. Herzberg, "Constants of Diatomic Molecules," Van Nostrand-Reinhold Co., New York, (1979).
- J. D. Cox, chairman, ICSU-CODATA Task Group on Key Values for Thermodynamics, *J. Chem. Thermodyn.* **10**, 903 (1978).
- G. A. Khachikurov, *Opt. Spectrosc.* **30**, 455 (1971).
- H. W. Woolley, R. B. Scott and F. G. Brickwedde, *J. Res. Nat. Bur. Stand.* **41**, 379 (1948).
- D. A. Shirley and W. F. Gianque, *J. Am. Chem. Soc.* **81**, 4778 (1959).
- G. P. Baxter, C. H. Hickley, and W. C. Holmes, *J. Am. Chem. Soc.* **29**, 127 (1907).
- J. J. Gillespie and M. R. Grosse, *J. Am. Chem. Soc.* **37**, 1061 (1915).
- T. H. Stern, Ph. D. Thesis, Univ. of Washington (1958).

TK	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ))/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>r</sub> H <sup>o</sup>	
0	0	0	-10.116	65.504	INFINITE
100	33.135	222.004	-7.080	65.489	-25.797
200	36.062	246.105	-6.403	65.489	-8.833
250	36.582	254.213	-1.769	63.240	-5.07
298.15	36.887	260.685	0	62.421	-3.386
300	36.897	260.913	0.068	62.388	-3.318
350	37.105	266.617	1.130	61.427	-1.777
400	37.256	271.582	2.138	59.460	-0.712
450	37.371	275.977	3.178	57.446	-0.082
457.666	37.386	276.609	3.631	55.930	---
500	37.464	279.920	4.681	54.300	---
600	37.612	286.764	6.783	51.269	---
700	37.735	292.571	8.983	48.000	---
800	37.847	297.618	11.269	44.500	---
900	37.959	302.082	13.646	40.800	---
1000	38.081	306.087	16.116	36.900	---
1100	38.232	309.724	18.683	32.800	---
1200	38.431	313.058	21.348	28.500	---
1300	38.699	316.084	24.113	24.000	---
1400	39.035	318.805	26.978	19.300	---
1500	39.507	321.734	29.943	14.500	---
1600	40.051	324.301	32.908	9.600	---
1700	40.674	326.747	35.873	4.700	---
1800	41.352	329.091	38.838	0	---
1900	42.054	331.346	41.803	0	---
2000	42.748	333.521	44.768	0	---
2100	43.404	335.622	47.733	0	---
2200	44.094	337.655	50.698	0	---
2300	44.819	339.622	53.663	0	---
2400	45.570	341.525	56.628	0	---
2500	46.343	343.363	59.593	0	---
2600	47.139	345.139	62.558	0	---
2700	47.958	346.851	65.523	0	---
2800	48.799	348.508	68.488	0	---
2900	49.661	350.088	71.453	0	---
3000	50.544	351.615	74.418	0	---
3100	51.448	353.082	77.383	0	---
3200	52.373	354.490	80.348	0	---
3300	53.319	355.842	83.313	0	---
3400	54.286	357.139	86.278	0	---
3500	55.274	358.384	89.243	0	---
3600	56.283	359.577	92.208	0	---
3700	57.313	360.723	95.173	0	---
3800	58.364	361.822	98.138	0	---
3900	59.436	362.877	101.103	0	---
4000	60.529	363.891	104.068	0	---
4100	61.644	364.864	107.033	0	---
4200	62.781	365.801	110.000	0	---
4300	63.940	366.701	112.965	0	---
4400	65.121	367.568	115.930	0	---
4500	66.324	368.404	118.895	0	---
4600	67.549	369.209	121.860	0	---
4700	68.796	369.986	124.825	0	---
4800	70.065	370.736	127.790	0	---
4900	71.356	371.460	130.755	0	---
5000	72.669	372.161	133.720	0	---
5100	74.004	372.838	136.685	0	---
5200	75.361	373.495	139.650	0	---
5300	76.740	374.130	142.615	0	---
5400	78.141	374.747	145.580	0	---
5500	79.564	375.345	148.545	0	---
5600	81.019	375.926	151.510	0	---
5700	82.506	376.490	154.475	0	---
5800	84.025	377.038	157.440	0	---
5900	85.576	377.572	160.405	0	---
6000	87.159	378.091	163.370	0	---

PREVIOUS September 1961 (1 atm)

CURRENT June 1982 (1 bar)

Iodine (I<sub>2</sub>)

I<sub>2</sub>(g)

Potassium Iodide ((KI)<sub>2</sub>)

IDEAL GAS

M<sub>r</sub> = 332.0056

S°(298.15 K) = [395.773] J·K<sup>-1</sup>·mol<sup>-1</sup> ΔH<sup>0</sup>(0 K) = -416.48 ± 4.2 kJ·mol<sup>-1</sup>  
 ΔH<sup>0</sup>(298.15 K) = -422.17 ± 4.2 kJ·mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies  
 ν, cm<sup>-1</sup> v, cm<sup>-1</sup>

[90](1)	[80](1)
[60](1)	[105](1)
[110](1)	[120](1)

Ground State Quantum Weight: [1]  
 Point Group: [D<sub>2h</sub>]

Bond Distances: K-I = [3.29] Å K-K = [4.00] Å

Bond Angles: K-I-K = [75°] I-K-I = [105°]

Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [5.073451] × 10<sup>-11</sup>] g<sup>3</sup>·cm<sup>6</sup>

σ = [4]

Enthalpy of Formation

The chemical equilibrium for the reaction K<sub>2</sub>I<sub>2</sub>(g) = 2 KI(g) has been studied by Datz and Datz *et al.*<sup>2</sup> They measured the temperature dependence of the molecular weight of KI(g) which was determined by measurement of the absolute pressure exerted by a known weight of completely vaporized salt contained in an isothermal fused silica bulb of known volume. Based on the reported P-V-T measurements, the enthalpy change of the reaction at 298.15 K is evaluated by the 2nd and 3rd law methods. The results are given in the table below.

Miller and Kusch determined the molecular composition of KI vapor by measurement of the velocity distribution of the molecules in the beam produced as the vapor effused through a small slit in a source. The analysis was based on an assumption that the velocity distribution within the oven is Maxwellian and that the vapor effuses through the ideal slit of kinetic theory. The velocity distributions of potassium and thallium atomic beams were found to be in excellent agreement with the theoretical distributions so the determination of the molecular composition of KI beams was tried. Using the derived equilibrium constants, we calculate the enthalpy change of the dissociation reaction by the 2nd and 3rd law methods. The results are presented in the following table.

The value of ΔH<sup>0</sup>(K<sub>2</sub>I<sub>2</sub>, g, 298.15 K) is adopted as -100.9 ± 1 kcal·mol<sup>-1</sup>.

Source	T/K	Data Points	ΔH <sup>0</sup> (298.15 K), kcal·mol <sup>-1</sup>	2nd law	3rd law	Drift	ΔH <sup>0</sup> (298.15 K) kcal·mol <sup>-1</sup>
Datz <sup>1</sup>	1226-1385	10	40.09 ± 0.82	40.66		0.4 ± 0.6	-100.66
	1292-1408	6	41.37 ± 1.91	41.01		-0.2 ± 1.4	-101.01
Miller Kusch <sup>2</sup>	816-921	10	54.62 ± 2.46	36.28		-21.4 ± 2.8	-96.28

Heat Capacity

The molecular structure and bond distance and angles were estimated by Berkowitz.<sup>4</sup> The vibrational frequencies are estimated by comparison with those calculated by Berkowitz and adjusted to give good agreement between 2nd and 3rd law evaluations of the equilibrium data. The three principal moments of inertia are: I<sub>A</sub> = 52.0871 × 10<sup>-39</sup>, I<sub>B</sub> = 287.1362 × 10<sup>-39</sup>, and I<sub>C</sub> = 339.2233 × 10<sup>-39</sup> g·cm<sup>2</sup>.

References

- <sup>1</sup>S. Datz, Oak Ridge National Laboratory, ORNL 2933, (1960).
- <sup>2</sup>S. Datz, W. T. Smith, Jr., and E. H. Taylor, *J. Chem. Phys.* **34**, 558 (1961).
- <sup>3</sup>R. C. Miller and P. Kusch, *J. Chem. Phys.* **25**, 860 (1956).
- <sup>4</sup>J. Berkowitz, *J. Chem. Phys.* **29**, 1386 (1958).
- <sup>5</sup>J. Berkowitz, *J. Chem. Phys.* **32**, 1519 (1960).

Potassium Iodide ((KI)<sub>2</sub>)

Enthalpy Reference Temperature = T<sub>r</sub> = 298.15 K

T/K	C <sub>p</sub> <sup>0</sup>	S° - (G° - H°(T <sub>r</sub> ))/T	H° - H°(T <sub>r</sub> )	kJ·mol <sup>-1</sup>	Standard State Pressure = P° = 0.1 MPa	log K <sub>r</sub>
0	0	INFINITE	-21.676	-416.480	-416.480	INFINITE
100	75.971	308.279	-15.972	-434.898	-434.898	227.167
200	81.203	363.113	-8.032	-419.471	-419.471	117.973
250	81.890	381.315	-3.953	-420.768	-420.768	96.032
298.15	82.258	395.772	0	-422.166	-422.166	81.812
300	82.268	396.281	0.152	-422.223	-422.223	81.356
350	82.499	408.982	4.272	-428.698	-428.698	70.805
400	82.649	420.008	9.007	-446.570	-446.570	62.719
450	82.752	429.749	12.536	-449.596	-449.596	56.218
500	82.826	438.472	16.675	-492.707	-492.707	50.586
600	82.973	453.583	24.963	-494.252	-494.252	41.995
700	82.982	466.370	33.259	-495.716	-495.716	35.839
800	83.040	477.453	41.559	-497.149	-497.149	31.209
900	83.046	487.233	49.862	-498.601	-498.601	27.597
1000	83.064	495.984	58.168	-500.123	-500.123	24.699
1100	83.078	503.901	66.475	-501.668	-501.668	21.882
1200	83.089	511.131	74.783	-503.350	-503.350	19.273
1300	83.097	517.792	83.093	-505.034	-505.034	17.065
1400	83.103	523.900	91.403	-506.789	-506.789	15.174
1500	83.109	529.674	99.713	-508.565	-508.565	13.536
1600	83.113	535.038	108.025	-510.363	-510.363	12.103
1700	83.116	540.076	116.336	-512.184	-512.184	10.839
1800	83.119	544.827	124.648	-514.029	-514.029	9.715
1900	83.122	549.321	132.960	-515.897	-515.897	8.709
2000	83.124	553.585	141.272	-517.787	-517.787	7.805
2100	83.126	557.641	149.585	-519.699	-519.699	6.986
2200	83.128	561.508	157.897	-521.633	-521.633	6.241
2300	83.129	565.203	166.210	-523.589	-523.589	5.561
2400	83.130	568.741	174.527	-525.567	-525.567	4.937
2500	83.131	572.135	182.836	-527.567	-527.567	4.362
2600	83.132	575.395	191.149	-529.589	-529.589	3.831
2700	83.133	578.533	199.463	-531.633	-531.633	3.339
2800	83.134	581.556	207.776	-533.698	-533.698	2.882
2900	83.135	584.473	216.089	-535.787	-535.787	2.456
3000	83.135	587.292	224.391	-537.899	-537.899	2.058
3100	83.136	590.018	232.717	-540.028	-540.028	1.685
3200	83.136	592.557	241.030	-542.174	-542.174	1.335
3300	83.137	595.215	249.344	-544.336	-544.336	1.006
3400	83.137	597.997	257.657	-546.514	-546.514	0.696
3500	83.138	600.107	265.971	-548.707	-548.707	0.403
3600	83.138	602.449	274.285	-550.914	-550.914	0.126
3700	83.138	604.727	282.589	-553.136	-553.136	-0.136
3800	83.139	606.944	290.815	-555.373	-555.373	-0.385
3900	83.139	609.104	299.217	-557.625	-557.625	-0.622
4000	83.139	611.209	307.340	-559.891	-559.891	-0.847
4100	83.139	613.262	315.854	-562.171	-562.171	-1.062
4200	83.140	615.265	324.168	-564.465	-564.465	-1.267
4300	83.140	617.221	332.482	-566.773	-566.773	-1.463
4400	83.140	619.133	340.796	-569.096	-569.096	-1.649
4500	83.140	621.001	349.110	-571.434	-571.434	-1.829
4600	83.140	622.829	357.424	-573.787	-573.787	-2.001
4700	83.140	624.617	365.738	-576.154	-576.154	-2.166
4800	83.141	626.367	374.052	-578.536	-578.536	-2.316
4900	83.141	628.081	382.366	-580.933	-580.933	-2.477
5000	83.141	629.761	390.681	-583.346	-583.346	-2.624
5100	83.141	631.407	398.995	-585.775	-585.775	-2.766
5200	83.141	633.022	407.309	-588.220	-588.220	-2.902
5300	83.141	634.605	415.623	-590.681	-590.681	-3.035
5400	83.141	636.160	423.937	-593.158	-593.158	-3.162
5500	83.141	637.685	432.251	-595.651	-595.651	-3.286
5600	83.142	639.183	440.565	-598.160	-598.160	-3.406
5700	83.142	640.655	448.879	-600.685	-600.685	-3.521
5800	83.142	642.101	457.194	-603.226	-603.226	-3.633
5900	83.142	643.522	465.508	-605.783	-605.783	-3.743
6000	83.142	644.919	473.822	-608.356	-608.356	-3.849

PREVIOUS: June 1967 (1 atm)

CURRENT: June 1967 (1 bar)

Potassium Iodide ((KI)<sub>2</sub>)

I<sub>2</sub>K<sub>2</sub>(g)



$I_2Li_2(g)$

$M_r = 267.6910$  Lithium Iodide ( $(LiI)_2$ )

IDEAL GAS

Lithium Iodide ( $(LiI)_2$ )

$\Delta H_f^\circ(0\text{ K}) = -356.74 \pm 16.7 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta H_f^\circ(298.15\text{ K}) = -361.92 \pm 16.7 \text{ kJ}\cdot\text{mol}^{-1}$

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
		S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	ΔH <sup>o</sup>	ΔG <sup>o</sup>	
0	0	INFINITE	-17.267	-356.740	-356.740	INFINITE
100	51.234	259.423	393.015	-356.873	-375.247	196.009
200	69.370	301.482	337.413	-359.315	-392.689	102.560
250	73.525	317.446	331.867	-360.618	-400.883	83.760
298.15	76.044	330.628	330.628	0	-408.522	71.571
300	76.121	331.098	330.629	0.141	-408.811	71.180
350	77.820	342.969	331.563	3.992	-416.504	62.160
400	78.982	353.441	333.656	7.914	-423.426	55.294
450	79.808	362.794	336.383	11.885	-428.552	49.745
500	80.414	371.235	339.453	15.891	-433.119	44.810
600	81.222	385.974	346.014	23.976	-437.940	37.256
700	81.720	398.535	352.642	31.125	-442.686	31.840
800	82.098	409.470	358.276	38.315	-447.239	27.765
900	82.375	419.147	363.224	48.531	-451.601	24.585
1000	82.458	427.825	371.057	56.767	-440.239	22.034
1100	82.559	435.688	376.581	63.018	-441.626	19.940
1200	82.652	442.876	381.810	73.278	-442.950	18.190
1300	82.724	449.494	386.766	81.547	-444.281	16.704
1400	82.782	455.627	391.468	89.823	-445.625	15.427
1500	82.828	461.340	395.938	98.103	-446.987	14.317
1600	82.866	466.687	400.194	106.388	-448.378	13.343
1700	82.898	471.712	404.255	114.676	-449.780	12.040
1800	82.924	476.451	408.135	122.968	-451.191	10.776
1900	82.947	480.935	411.850	131.261	-452.614	9.645
2000	82.966	485.190	415.412	139.557	-454.053	8.628
2100	82.983	489.238	418.832	147.854	-455.507	7.707
2200	82.997	493.099	422.120	156.153	-456.976	6.869
2300	83.009	496.782	425.287	164.454	-458.459	6.104
2400	83.020	500.322	428.340	172.754	-459.954	5.405
2500	83.030	503.711	431.288	181.058	-461.464	4.757
2600	83.039	506.968	434.136	189.361	-462.987	4.161
2700	83.046	510.102	436.892	197.665	-464.523	3.608
2800	83.053	513.122	439.561	205.970	-466.071	3.095
2900	83.059	516.037	442.148	214.276	-467.634	2.616
3000	83.065	518.852	444.658	222.582	-469.216	2.169
3100	83.070	521.576	447.096	230.889	-470.818	1.751
3200	83.074	524.214	449.465	239.196	-472.439	1.359
3300	83.079	526.770	451.769	247.504	-474.074	0.990
3400	83.082	529.250	454.012	255.812	-475.724	0.642
3500	83.086	531.659	456.196	264.120	-477.389	0.315
3600	83.089	533.999	458.325	272.429	-479.069	0.005
3700	83.092	536.276	460.401	280.738	-480.764	-0.289
3800	83.095	538.492	462.427	289.047	-482.475	-0.597
3900	83.097	540.650	464.405	297.357	-484.203	-0.881
4000	83.099	542.754	466.338	305.667	-485.957	-1.082
4100	83.102	544.806	468.226	313.977	-487.739	-1.321
4200	83.104	546.809	470.074	322.287	-489.549	-1.548
4300	83.105	548.764	471.881	330.597	-491.384	-1.766
4400	83.107	550.675	473.650	338.908	-493.244	-1.973
4500	83.109	552.542	475.383	347.219	-495.129	-2.171
4600	83.110	554.369	477.080	355.530	-497.039	-2.361
4700	83.112	556.157	478.744	363.841	-498.974	-2.543
4800	83.113	557.906	480.375	372.152	-500.934	-2.718
4900	83.114	559.620	481.974	380.464	-502.919	-2.886
5000	83.116	561.299	483.544	388.775	-504.929	-3.047
5100	83.117	562.945	485.083	397.087	-506.964	-3.202
5200	83.118	564.559	486.598	405.398	-509.024	-3.351
5300	83.119	566.142	488.084	413.710	-511.109	-3.494
5400	83.120	567.696	489.544	422.022	-513.219	-3.633
5500	83.120	569.221	490.979	430.334	-515.354	-3.766
5600	83.121	570.719	492.389	438.646	-517.514	-3.896
5700	83.122	572.190	493.776	446.958	-519.699	-4.020
5800	83.123	573.636	495.141	455.271	-521.909	-4.141
5900	83.124	575.057	496.483	463.583	-524.144	-4.258
6000	83.124	576.454	497.805	471.895	-526.404	-4.371

CURRENT June 1966 (1 bar)

PREVIOUS June 1966 (1 atm)

Lithium Iodide ( $(LiI)_2$ )

$I_2Li_2(g)$

Vibrational Frequencies and Degeneracies  
 $\nu$ , cm<sup>-1</sup> [310](1)  
 [160](1) 248 (1)  
 [383](1) 375 (1)

Ground State Quantum Weight: 1  
 $\sigma = 4$

Bond Distances: Li-I = 2.54 Å; Li-Li = 2.71 Å  
 Bond Angles: I-Li-I = 116° ± 4°; Li-I-Li = 64°  
 Product of the Moments of Inertia:  $I_A I_B I_C = 1.631229 \times 10^{-112} \text{ g}^3 \cdot \text{cm}^6$

**Enthalpy of Formation**  
 This was obtained from the enthalpy of formation of the crystal and the enthalpy of sublimation to the dimer, which derivation has been given in the LiI(g) table.

**Heat Capacity and Entropy**  
 Berkowitz has calculated the molecular structure and vibrational frequencies based on the ionic model. The planar rhombic structure proposed by Berkowitz has been confirmed by the lack of polarity in electric deflection by Buchler *et al.* The selected bond distances and  $r(Li-Li) = 2.712 \text{ \AA}$  and  $r(I-Li) = 4.520 \text{ \AA}$ , calculated by Berkowitz are in good agreement with those from Akischin and Rambidi.<sup>3</sup> The principal moments of inertia are:  $I_A = 4.1763 \times 10^{-39} \text{ g} \cdot \text{cm}^2$ ,  $I_B = 195.5561 \times 10^{-39} \text{ g} \cdot \text{cm}^2$ , and  $I_C = 199.7324 \times 10^{-39} \text{ g} \cdot \text{cm}^2$ .

Bauer *et al.* have estimated six vibrational frequencies (501, 501, 148, 200, 294, 360 cm<sup>-1</sup>) for Li<sub>2</sub>I<sub>2</sub>(g) in the electron diffraction studies of the Li<sub>2</sub>Cl<sub>2</sub>(g) Klemperer and Norris have observed two fundamental vibrational frequencies (248 and 375 cm<sup>-1</sup>) in the infrared spectrum and tentatively assigned them as B<sub>2g</sub> and B<sub>2u</sub> modes; these have been adopted in the tabulation. The remaining four vibrational frequencies were obtained from Berkowitz because his model and derivation are self consistent.

**References**  
<sup>1</sup>J. Berkowitz, *J. Chem. Phys.* **29**, 1386 (1958), **32**, 1519 (1960).  
<sup>2</sup>A. Buchler, J. L. Stauffer and W. Klemperer, *J. Amer. Chem. Soc.* **86**, 4544 (1964).  
<sup>3</sup>P. A. Akischin and N. G. Rambidi, *Z. Physik. Chem.* **213**, 111 (1960).  
<sup>4</sup>S. H. Bauer, T. Ino and R. F. Porter, *J. Chem. Phys.* **33**, 685 (1960).  
<sup>5</sup>W. Klemperer and W. G. Norris, *J. Chem. Phys.* **34**, 1071 (1961).

I<sub>2</sub>Mg<sub>1</sub>(cr)Magnesium Iodide (MgI<sub>2</sub>)M<sub>r</sub> = 278.1140

## CRYSTAL

Magnesium Iodide (MgI<sub>2</sub>)

S<sup>o</sup>(298.15 K) = [129 704 ± 4.2] J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>fus</sub> = 907 ± 15 K  
 $\Delta H_f^o(0 \text{ K}) = \text{Unknown}$   
 $\Delta H_f^o(298.15 \text{ K}) = -366.94 \pm 6.3 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{sub}}H^o = 29\,288 \pm 8.4 \text{ kJ}\cdot\text{mol}^{-1}$

## Enthalpy of Formation

Finch *et al.*<sup>1</sup> measured the enthalpy of solution of MgO(cr) in aqueous HI and of MgI<sub>2</sub>(cr) in the same solvent. Combining and correcting for a concentration change gives  $\Delta H_f^o(298.15 \text{ K}) = 14.53 \text{ kcal}\cdot\text{mol}^{-1}$  for the process MgO(cr) + 2 HI(0.5m) = MgI<sub>2</sub>(cr) + H<sub>2</sub>O(l) from which  $\Delta H_f^o(\text{MgI}_2, \text{cr}, 298.15 \text{ K}) = -87.70 \pm 1.5 \text{ kcal}\cdot\text{mol}^{-1}$  is calculated. The auxiliary data used are  $\Delta H_f^o(\text{MgO}, \text{cr}, 298.15 \text{ K}) = -143.7 \text{ kcal}\cdot\text{mol}^{-1}$ ,  $\Delta H_f^o(\text{H}_2\text{O}, \text{l}, 298.15 \text{ K}) = -68.315 \text{ kcal}\cdot\text{mol}^{-1}$ , and  $\Delta H_f^o(\text{HI}, 0.5\text{m}, 298.15 \text{ K}) = -13.42 \text{ kcal}\cdot\text{mol}^{-1}$ . This last value was calculated from the CODATA value of -13.60 for  $\Delta H_f^o(\text{HI}, \text{aq}, \text{std. state}, 298.15 \text{ K}) = \Delta H_f^o(\text{HI}, \text{aq}, \text{std. state}, 298.15 \text{ K})$  and the enthalpy of dilution of HI.<sup>4</sup>

Combination of  $\Delta H_f^o(\text{Mg}^{2+}, \text{aq}, \text{std. state}, 298.15 \text{ K}) = -111.58 \text{ kcal}\cdot\text{mol}^{-1}$ , selected by Parker<sup>4,5</sup> with the CODATA value of  $\Delta H_f^o(\text{I}, \text{aq}, \text{std. state}, 298.15 \text{ K}) = -13.60 \text{ kcal}\cdot\text{mol}^{-1}$  gives  $\Delta H_f^o(\text{MgI}_2, \text{aq}, \text{std. state}, 298.15 \text{ K}) = -138.78 \text{ kcal}\cdot\text{mol}^{-1}$ . Further combination with the enthalpy of solution, -50.96 kcal·mol<sup>-1</sup>,<sup>4</sup> gives  $\Delta H_f^o(\text{MgI}_2, \text{cr}, 298.15 \text{ K}) = -87.82 \text{ kcal}\cdot\text{mol}^{-1}$ . We adopt  $\Delta H_f^o(\text{MgI}_2, \text{cr}, 298.15 \text{ K}) = -87.7 \pm 1.5 \text{ kcal}\cdot\text{mol}^{-1}$  to retain internal consistency.

## Heat Capacity and Entropy

$C_p^o(298.15 \text{ K}) = 17.88 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  is calculated from the reaction MgCl<sub>2</sub>(cr) + 2 NaI(cr) = MgI<sub>2</sub>(cr) + 2 NaCl(cr) assuming no net change in heat capacity.  $C_p^o = 21.0 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  at T<sub>fus</sub> = 907 K estimated from a Kopp's rule value of 7.0 cal·K<sup>-1</sup>·g atom appears reasonable in comparison with a  $C_p^o$  vs. T plot for MgBr<sub>2</sub>(cr), MgCl<sub>2</sub>(cr) and CaI<sub>2</sub>(cr).<sup>2</sup> Values of  $C_p^o$  between 298.15 and 907 K are read from the graphical comparison curve. The adopted values lead to  $H^o(500 \text{ K}) - H^o(298.15 \text{ K}) = 3.77 \text{ kcal}\cdot\text{mol}^{-1}$ , in reasonable agreement with the estimate of 4.0 by Brewer *et al.*<sup>6</sup>

S<sup>o</sup>(298.15 K) = 31.0 ± 1.0 cal·K<sup>-1</sup>·mol<sup>-1</sup> is adopted from Kelley and King.<sup>7</sup>

## Fusion Data

The melting point of 650 °C (923 K) quoted in the literature appears to be based on the assumed value of Devoto and Jeny<sup>8</sup> in a study of molten electrolytes, Bockris *et al.*<sup>9</sup> found MgI<sub>2</sub> to be molten at 910 K; a graph in the same paper infers that a T<sub>fus</sub> = 907 K was chosen. We adopt T<sub>fus</sub> = 907 ± 15 K.

From the K/MgI<sub>2</sub> phase diagram by Klemm *et al.*<sup>10</sup> values of  $\Delta_{\text{sub}}H^o(\text{MgI}_2)$  ranging from 7 to 9 kcal·mol<sup>-1</sup> are calculated. Brewer<sup>11</sup> earlier estimated 5.3 kcal·mol<sup>-1</sup>. We adopt 7.0 ± 2.0 kcal·mol<sup>-1</sup>.

## Sublimation Data

By a mass spectrometric-Knudsen cell technique, Berkowitz and Marguard<sup>12</sup> found the sublimation pressure of MgI<sub>2</sub>(cr) to be 5.18 × 10<sup>-6</sup> atm at 734 K and 2.02 × 10<sup>-5</sup> atm at 757 K. A 3rd law analysis of these two points gives  $\Delta_{\text{sub}}H^o(298.15 \text{ K}) = 49.4 \pm 0.8 \text{ kcal}\cdot\text{mol}^{-1}$ . The 2nd law analysis of these two points gives 67.5 kcal·mol<sup>-1</sup> but other data covering an approximate range of 550 to 750 K are shown graphically by Berkowitz and Marguard<sup>12</sup> from which they calculate  $\Delta_{\text{sub}}H^o(550-750 \text{ K}) = 45 \text{ kcal}\cdot\text{mol}^{-1}$ . We adopt  $\Delta_{\text{sub}}H^o(298.15 \text{ K}) = 49.4 \pm 0.8 \text{ kcal}\cdot\text{mol}^{-1}$ .

## References

1. A. Finch, P. J. Gardner, and C. J. Steadman, *Can. J. Chem.* **46**, 3447 (1968).
2. JANAF Thermochemical Tables: MgO(cr), 12-31-74; MgBr<sub>2</sub>(cr), 6-30-74; MgCl<sub>2</sub>(cr), 12-31-65; CaCl<sub>2</sub>(cr), 6-30-70.
3. J. D. Cox, ICSU CODATA Task Group on Key Values for Thermodynamics, *J. Chem. Thermodyn.* **4**, 331 (1972).
4. U. S. Nat. Bur. Stand. Tech. Note 270-3, 264 pp. (1968).
5. V. B. Parker, U. S. Nat. Bur. Stand. Report 9803, (1968).
6. L. Brewer, L. A. Bromley, P. W. Gilles, and N. L. Loifgren in "The Chemistry and Metallurgy of Miscellaneous Materials, Thermodynamics," L. L. Quill, Ed., McGraw Hill, New York, (1950).
7. K. K. Kelley and E. G. King, U. S. Bur. Mines Bull. 592, 149 pp. (1961).
8. G. Devoto and G. Jeny, *Gazz. Chim., Ital.* **61**, 305 (1931).
9. J. O'M. Bockris, E. H. Crook, H. Bloom and N. E. Richards, *Proc. Roy. Soc. (London)* **A255**, 558 (1960).
10. W. Klemm, K. Beyersdorfer, and J. Oryschkewitsch, *Z. anorg. allg. Chem.* **256**, 34 (1948).
11. L. Brewer in "The Chemistry and Metallurgy of Miscellaneous Materials, Thermodynamics," L. L. Quill, Ed., McGraw Hill, New York, (1950).
12. J. Berkowitz and J. R. Marquart, *J. Chem. Phys.* **37**, 1853 (1962).

PREVIOUS.

CURRENT December 1974

Magnesium Iodide (MgI<sub>2</sub>)I<sub>2</sub>Mg<sub>1</sub>(cr)

**I<sub>2</sub>MgI(l)**

**M<sub>r</sub> = 278.1140 Magnesium Iodide (MgI<sub>2</sub>)**

**LIQUID**

**Magnesium Iodide (MgI<sub>2</sub>)**

$S^{\circ}(298.15\text{ K}) = [155.737] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = 907 \pm 15 \text{ K}$

$\Delta H^{\circ}(298.15\text{ K}) = [-342.252] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{fus}}H^{\circ} = 29.288 \pm 8.4 \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**

$\Delta H^{\circ}(\text{MgI}_2, \text{l}, 298.15\text{ K})$  is calculated from  $\Delta H^{\circ}(\text{MgI}_2, \text{cr}, 298.15\text{ K})$  by adding the enthalpy of fusion,  $\Delta_{\text{fus}}H^{\circ}$ , and the difference in enthalpy,  $H^{\circ}(907\text{ K}) - H^{\circ}(298.15\text{ K})$ , between the crystal and the liquid.

**Heat Capacity and Entropy**

The liquid heat capacity of  $24.0 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  (8 cal·K<sup>-1</sup>·g-atom) follows the trend of the liquid heat capacities of the alkaline earth chlorides and bromides and the other alkaline earth iodides. This value is adopted and assumed constant over a 600–2000 K range. A glass transition is assumed at 600 K below which the heat capacity is that of the crystal.

$S^{\circ}(\text{MgI}_2, \text{l}, 298.15\text{ K})$  is calculated in a manner similar to that used for the enthalpy of formation.

**Fusion Data**

Refer to the crystal table for details.

**Vaporization Data**

$T_{\text{vap}} = 1255 \text{ K}$  is calculated as the temperature at which the fugacity is 1 atm for the reaction  $\text{MgI}_2(\text{l}) = \text{MgI}_2(\text{g})$ .  $\Delta_{\text{vap}}H^{\circ} = 36.126 \text{ kcal}\cdot\text{mol}^{-1}$  is the calculated difference between the enthalpies of formation of the ideal gas and the liquid at  $T_{\text{vap}}$ .

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	ΔH <sup>o</sup>	
0					
100					
200					
298.15	74.810	155.737	0.	-342.252	60.323
300	74.977	155.738	0.139	-342.260	59.953
400	78.408	158.723	7.815	-358.776	44.973
500	80.919	196.035	15.785	-401.669	35.172
600	83.011	210.980	23.985	-399.991	28.192
600.000	83.011	210.980	23.985	GLASS <- -> LIQUID	
600.000	100.416	171.004	23.985	TRANSITION	
700	100.416	226.459	34.027	-396.589	23.237
800	100.416	239.867	44.068	-393.315	19.553
900	100.416	251.695	54.110	-390.182	16.710
907.000	100.416	252.473	54.813	CRYSTAL <- -> LIQUID	
1000	100.416	262.275	64.152	-395.798	14.417
1100	100.416	271.845	74.193	-393.003	12.544
1200	100.416	280.583	84.235	-390.225	10.994
1300	100.416	288.620	94.276	-387.470	9.692
1400	100.416	296.062	104.318	-512.156	8.465
1500	100.416	302.990	114.360	-508.120	7.196
1600	100.416	309.471	124.401	-504.134	6.095
1700	100.416	315.558	134.443	-500.207	5.130
1800	100.416	321.298	144.484	-496.345	4.280
1900	100.416	326.727	154.526	-492.552	3.525
2000	100.416	331.878	164.568	-488.850	2.850

PREVIOUS:

CURRENT December 1974

**Magnesium Iodide (MgI<sub>2</sub>)**

**I<sub>2</sub>MgI(l)**

$I_2Mg_1(cr,l)$

$M_r = 278.1140$  Magnesium Iodide ( $MgI_2$ )

CRYSTAL-LIQUID

Magnesium Iodide ( $MgI_2$ )

0 to 907 K crystal  
above 907 K liquid

Refer to the individual tables for details.

T/K	$C_p^*$	Enthalpy Reference Temperature = $T_r = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa		$\log K_f$
		$J \cdot K^{-1} \cdot mol^{-1}$	$S^\circ - [G^\circ - H^\circ(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	
0						
100						
200						
298.15	74.810	129.704	129.704	0	-366.937	63.288
300	74.977	130.167	129.705	0.139	-366.945	62.891
400	78.408	152.229	132.690	7.815	-383.462	46.836
500	80.919	170.002	138.432	15.785	-426.355	36.391
600	83.011	184.946	144.971	23.983	-424.677	28.981
700	84.726	197.873	151.626	32.373	-422.928	23.710
800	86.274	209.290	158.134	40.925	-421.144	19.773
900	87.653	219.502	164.395	49.596	-419.381	16.723
907.000	87.864	220.182	164.823	50.210	CRYSTAL $\leftarrow$ LIQUID	
907.000	100.416	252.473	164.823	79.498	TRANSITION	
1000	100.416	262.275	173.438	88.837	-395.798	14.417
1100	100.416	271.845	181.956	98.879	-393.003	12.544
1200	100.416	280.583	189.816	108.920	-390.225	10.994
1300	100.416	288.620	197.111	118.962	-387.470	9.692
1400	100.416	296.062	203.917	129.003	-384.740	8.465
1500	100.416	302.990	210.293	139.045	-382.040	7.196
1600	100.416	309.471	216.291	149.087	-379.369	6.095
1700	100.416	315.558	221.953	159.128	-376.722	5.130
1800	100.416	321.298	227.315	169.170	-374.101	4.280
1900	100.416	326.727	232.405	179.211	-371.512	3.525
2000	100.416	331.878	237.251	189.253	-368.950	2.850

PREVIOUS.

CURRENT December 1974

Magnesium Iodide ( $MgI_2$ )

$I_2Mg_1(cr,l)$

**I<sub>2</sub>Mg<sub>l</sub>(g)**

**Magnesium Iodide (MgI<sub>2</sub>)**

**IDEAL GAS**

**Magnesium Iodide (MgI<sub>2</sub>)**

T/K	Enthalpy Reference Temperature = T, $\sigma = 298.15$ K		Standard State Pressure = $p^\circ = 0.1$ MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	$\Delta_f H^\circ$	
0	0	0	INFINITE	INFINITE	INFINITE
100	51.832	256.256	157.563	-157.563	-175.563
200	57.298	294.115	156.990	-156.990	-175.566
250	58.718	307.064	158.436	-158.436	-193.639
298.15	59.623	317.489	159.332	-159.332	-202.337
300	59.651	317.490	160.247	-160.247	-210.538
350	60.281	327.104	160.284	-160.284	-210.850
400	60.721	335.183	161.359	-161.359	-219.196
450	61.038	342.355	178.452	-178.452	-226.834
500	61.273	348.798	180.762	-180.762	-232.743
600	61.590	360.000	223.213	-223.213	-234.595
700	61.787	369.510	223.590	-223.590	-236.838
800	61.917	377.770	224.060	-224.060	-239.010
900	62.008	385.068	224.641	-224.641	-241.108
1000	62.073	391.603	225.354	-225.354	-243.125
1100	62.122	397.523	226.168	-226.168	-245.142
1200	62.159	402.930	227.044	-227.044	-247.159
1300	62.189	407.907	228.000	-228.000	-249.176
1400	62.212	412.517	229.046	-229.046	-251.193
1500	62.230	416.809	230.282	-230.282	-253.210
1600	62.246	420.826	231.700	-231.700	-255.227
1700	62.259	424.600	233.300	-233.300	-257.244
1800	62.269	428.159	235.075	-235.075	-259.261
1900	62.278	431.526	237.015	-237.015	-261.278
2000	62.286	434.721	239.105	-239.105	-263.295
2100	62.293	437.760	241.340	-241.340	-265.312
2200	62.298	440.655	243.715	-243.715	-267.329
2300	62.304	443.407	246.225	-246.225	-269.346
2400	62.308	446.019	248.865	-248.865	-271.363
2500	62.312	448.523	251.630	-251.630	-273.380
2600	62.315	451.067	254.525	-254.525	-275.397
2700	62.318	453.648	257.545	-257.545	-277.414
2800	62.321	456.265	260.685	-260.685	-279.431
2900	62.324	458.925	263.940	-263.940	-281.448
3000	62.326	461.625	267.305	-267.305	-283.465
3100	62.328	464.360	270.785	-270.785	-285.482
3200	62.330	467.135	274.375	-274.375	-287.499
3300	62.332	469.955	278.070	-278.070	-289.516
3400	62.333	472.815	281.865	-281.865	-291.533
3500	62.334	475.710	285.765	-285.765	-293.550
3600	62.336	478.635	289.765	-289.765	-295.567
3700	62.337	481.590	293.860	-293.860	-297.584
3800	62.338	484.570	298.045	-298.045	-299.601
3900	62.339	487.575	302.320	-302.320	-301.618
4000	62.340	490.600	306.685	-306.685	-303.635
4100	62.341	493.645	311.135	-311.135	-305.652
4200	62.342	496.710	315.670	-315.670	-307.669
4300	62.342	499.795	320.285	-320.285	-309.686
4400	62.343	502.900	324.975	-324.975	-311.703
4500	62.344	506.020	329.740	-329.740	-313.720
4600	62.344	509.155	334.575	-334.575	-315.737
4700	62.345	512.310	339.480	-339.480	-317.754
4800	62.346	515.480	344.445	-344.445	-319.771
4900	62.346	518.660	349.470	-349.470	-321.788
5000	62.347	521.855	354.550	-354.550	-323.805
5100	62.347	525.060	359.685	-359.685	-325.822
5200	62.347	528.275	364.870	-364.870	-327.839
5300	62.348	531.500	370.110	-370.110	-329.856
5400	62.348	534.735	375.400	-375.400	-331.873
5500	62.349	538.000	380.740	-380.740	-333.890
5600	62.349	541.285	386.130	-386.130	-335.907
5700	62.349	544.590	391.570	-391.570	-337.924
5800	62.349	547.910	397.060	-397.060	-339.941
5900	62.350	551.245	402.600	-402.600	-341.958
6000	62.350	554.590	408.190	-408.190	-343.975

$\Delta_f H^\circ(0\text{ K}) = -157.56 \pm 10.5\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = -160.25 \pm 10.5\text{ kJ}\cdot\text{mol}^{-1}$

Vibrational Frequencies and Degeneracies  
 $\nu$ ,  $\text{cm}^{-1}$   
 [125](1)  
 [60](2)  
 [423](1)

Ground State Quantum Weight: [1]  
 Point Group: D<sub>∞h</sub>  
 Bond Distance: Mg-I = 2.52 ± 0.03 Å  
 Bond Angle: I-Mg-I = 180°  
 Rotational Constant: B<sub>0</sub> = [0.010459] cm<sup>-1</sup>

**Enthalpy of Formation**

$\Delta_f H^\circ(\text{MgI}_2, g, 298.15\text{ K})$  is obtained from that of the crystal by addition of  $\Delta_{\text{sub}} H^\circ(298.15\text{ K}) = 49.4 \pm 0.8\text{ kcal}\cdot\text{mol}^{-1}$ . The enthalpy of sublimation is derived from the sublimation pressure measurements of Berkowitz and Marquart.<sup>1</sup> Refer to the MgI<sub>2</sub>(Cr) table.

**Heat Capacity and Entropy**

The bond distance is taken from the electron diffraction study of Akishin and Spiridonov.<sup>2</sup> From an electric deflection study of mass spectrometrically detected molecular beams, Buechler *et al.*<sup>3</sup> concluded that MgI<sub>2</sub> is linear. The equality of the stretching force constant of the alkaline earth monohalide and the stretching force constant of the alkaline earth dihalide has been indicated as a reasonable assumption.<sup>4,5</sup> The stretching force constant for MgI(g) is calculated, using the valence force model, from the ground state vibrational frequency given by Rosen.<sup>6</sup> The bending force constant for MgI(g) is taken as 0.01 of the stretching force constant. Brewer *et al.*<sup>4</sup> used a factor of 0.1 for MgI<sub>2</sub>; however, a factor of 0.01 appears more reasonable.<sup>7</sup> The adopted vibrational frequencies are calculated from the estimated force constants. Other estimates for  $\nu_1$ ,  $\nu_2$ , and  $\nu_3$  are 132, 199, 446<sup>4</sup> and 137, 140, 464.<sup>8</sup> We assign an uncertainty of ± 2 cal·K<sup>-1</sup>·mol<sup>-1</sup> to the entropy to allow for error in estimating the vibrational frequencies.

**References**

- <sup>1</sup>J. Berkowitz and J. R. Marquart, *J. Chem. Phys.* **37**, 1853 (1962).
- <sup>2</sup>P. A. Akishin and V. P. Spiridonov, *Zhur. Fiz. Khim.* **32**, 1682 (1958).
- <sup>3</sup>A. Buechler, J. L. Stauffer and W. Klemperer, *J. Amer. Chem. Soc.* **86**, 4544 (1964).
- <sup>4</sup>L. Brewer, G. R. Somayajulu, and E. Brackett, *Chem. Rev.* **63**, 111 (1963).
- <sup>5</sup>JANAF Thermochemical Tables: BeF<sub>2</sub>(g), 6-30-70; MgF<sub>2</sub>(g), 12-31-68; CaF<sub>2</sub>(g), 12-31-72; BaF<sub>2</sub>(g), 12-31-72; CaI<sub>2</sub>(g), 6-30-74; SrI<sub>2</sub>(g), 6-30-74; BaI<sub>2</sub>(g), 6-30-74.
- <sup>6</sup>B. Rosen, Ed., "Spectroscopic Data Relative to Diatomic Molecules," Pergamon Press, New York, (1970).
- <sup>7</sup>JANAF Thermochemical Table: MgBr<sub>2</sub>(g), 6-30-74.
- <sup>8</sup>K. S. Krasnov and V. I. Svetsov, *Izv. Vysshikh Uchebn. Zavedenii, Khim. i Khim. Tekhnol.* **6**, 167 (1963).

PREVIOUS December 1974 (1 atm) CURRENT: December 1974 (1 bar)

**Magnesium Iodide (MgI<sub>2</sub>)**

**Molybdenum Iodide ( $\alpha$ -MoI<sub>2</sub>)**      **CRYSTAL ( $\alpha$ )**       **$M_r = 349.7490$**       **Molybdenum Iodide, Alpha (MoI<sub>2</sub>)**      **I<sub>2</sub>Mo<sub>1</sub>(cr)**

$S^\circ(298.15 \text{ K}) = [149.662 \pm 16.7] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$   
 $T_{\text{trans}} = 1305 \text{ K}$  (total  $p = 1 \text{ atm}$ )

$\Delta_f H^\circ(0 \text{ K}) = \text{Unknown}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = -103.93 \pm 12.6 \text{ kJ mol}^{-1}$

#### Enthalpy of Formation

Barnes *et al.*<sup>1</sup> have measured calorimetrically the enthalpy of formation of MoI<sub>2,3</sub> by reacting iodine vapor with Mo(CO)<sub>6</sub> at 539 K. The products were shown to consist of MoI<sub>3</sub>, MoI<sub>2</sub>, and Mo by chemical analysis. Assuming a difference in the enthalpies of formation of MoI<sub>3</sub> and MoI<sub>2</sub> of  $-1.5 \text{ kcal} \cdot \text{mol}^{-1}$ , Barnes *et al.*<sup>1</sup> determined  $\Delta_f H^\circ(\text{MoI}_2, \text{cr}, 298.15 \text{ K}) = -24.7 \pm 2 \text{ kcal mol}^{-1}$ . Brewer<sup>2</sup> has estimated that the difference  $\Delta_f H^\circ(\text{MoI}_3) - \Delta_f H^\circ(\text{MoI}_2)$  may be as large as  $-5 \text{ kcal mol}^{-1}$ , and he reanalyzed the enthalpy of iodination data with the result  $\Delta_f H^\circ(\text{MoI}_2, \text{cr}, 298.15 \text{ K}) = -12500 \pm 1500 \text{ KJ/R} = -12500 \pm 1500 \text{ K}$  which is adopted. The assigned uncertainty ( $\pm 3 \text{ kcal mol}^{-1}$ ) is determined from the product 1500xR which has been rounded to the nearest kcal·mol<sup>-1</sup>.

#### Heat Capacity and Entropy

Values of  $S^\circ(298.15 \text{ K})$  and  $C_p^\circ$  over the temperature range 298–1500 K are estimates reported by Brewer.<sup>2</sup> We treat his reported value of  $S^\circ(298.15 \text{ K})$  in a manner similar to that for the heat of formation.

#### Phase Data

The crystal structure<sup>3</sup> of  $\alpha$ -MoI<sub>2</sub> in the Pearson classification system of *oC72*. Glicksman and Walton<sup>3</sup> have reported preparing a new molybdenum diiodide phase ( $\beta$ -MoI<sub>2</sub>) by reacting Mo<sub>2</sub>(O<sub>2</sub>CCH<sub>3</sub>)<sub>4</sub> with HI gas at 573 K. We assume that this new phase is unstable with respect to  $\alpha$ -MoI<sub>2</sub> at all temperatures.

#### Decomposition Data

$T_{\text{trans}}$  is calculated as the temperature at which the partial pressures of I<sub>2</sub>(g) and I(g) reach one atmosphere over crystalline MoI<sub>2</sub> and Mo. At  $T_{\text{trans}} = 1305 \text{ K}$ , we calculate the vapor composition to consist of 0.63 atm of I<sub>2</sub> and 0.37 atm of I. Saturated vapor pressure measurements by Drobot *et al.*<sup>4</sup> on MoI<sub>2</sub>(cr) prepared by thermal decomposition of MoI<sub>3</sub>(cr) show that initial decomposition to the metal and iodine occurs at 1063 K and 0.33 atm.

#### References

- <sup>1</sup>D. S. Barnes, G. Plicher, D. A. Pittam, H. A. Skinner, D. Todd, and Y. Virmani, *J. Less Common Met.* **6**, 177 (1974).
- <sup>2</sup>L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal communication, September 28, 1978, preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria.
- <sup>3</sup>H. D. Glicksman and R. A. Walton, *Inorg. Chem.* **7**, 200 (1978).
- <sup>4</sup>D. V. Drobot, L. G. Mikhalova, K. A. Bol'shakov, and V. L. Sbitnev, *Russ. J. Inorg. Chem.* **3**, 643 (1978).

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa	
		S <sup>o</sup> - (G <sup>o</sup> - fF <sup>o</sup> (T <sub>r</sub> ))/T	H <sup>o</sup> - fF <sup>o</sup> (T <sub>r</sub> )	Δ <sub>f</sub> H <sup>o</sup>	Δ <sub>f</sub> G <sup>o</sup>
0					
100					
200					
298.15	82.705	149.662	0	-103.931	-105.396
300	82.730	149.663	0.153	-103.923	-105.405
400	83.977	152.923	8.488	-119.681	-105.390
500	85.224	159.120	16.948	-161.966	-97.768
600	86.471	166.110	25.533	-159.752	-85.135
700	87.718	173.171	34.243	-157.483	-72.878
800	88.964	180.057	43.077	-155.149	-60.950
900	90.211	186.616	52.035	-152.747	-49.318
1000	91.458	192.884	61.119	-150.278	-37.958
1100	92.705	198.844	70.377	-147.748	-26.848
1200	93.952	204.515	79.660	-145.166	-15.971
1300	95.199	209.915	88.117	-142.546	-3.510
1400	96.445	215.068	98.700	-139.890	1.147
1500	97.696	219.993	108.407	-137.246	13.415

PREVIOUS:

CURRENT: September 1978

Molybdenum Iodide, Alpha (MoI<sub>2</sub>)I<sub>2</sub>Mo<sub>1</sub>(cr)

I<sub>2</sub>Mo<sub>2</sub>(g)

M<sub>r</sub> = 349.7490 Molybdenum Iodide (MoI<sub>2</sub>)

IDEAL GAS

Molybdenum Iodide (MoI<sub>2</sub>)

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	Δ <sub>f</sub> H°	
0	0	INFINITE	-18.140	257.377	INFINITE
100	61.708	265.272	400.919	238.686	-124.677
200	69.265	311.318	345.722	218.944	-57.182
250	70.171	326.880	340.452	209.128	-43.693
298.15	70.717	339.290	339.290	199.734	-34.992
300	70.733	339.728	339.291	199.372	-34.714
350	71.082	350.660	340.154	189.682	-28.308
400	71.254	360.164	342.074	180.614	-23.586
450	71.268	368.559	344.560	173.204	-20.105
500	71.146	376.063	347.342	169.786	-17.737
600	70.599	388.991	353.240	164.252	-14.299
700	69.827	399.818	359.142	158.600	-11.833
800	68.958	409.087	364.820	152.893	-9.883
900	68.198	417.167	370.197	149.136	-8.239
1000	67.478	424.314	375.258	144.332	-7.382
1100	66.847	430.715	380.014	139.530	-6.436
1200	66.305	436.508	384.484	134.731	-5.647
1300	65.842	441.796	388.692	129.944	-4.980
1400	65.449	446.661	392.662	125.181	-4.409
1500	65.118	451.165	396.414	120.450	-3.916
1600	64.840	455.338	399.968	115.758	-3.485
1700	64.609	459.282	403.343	111.115	-3.107
1800	64.422	463.020	406.554	106.524	-2.772
1900	64.272	466.449	409.616	102.004	-2.474
2000	64.157	469.742	412.540	97.567	-2.208
2100	64.075	472.870	415.339	93.211	-1.969
2200	64.022	475.850	418.025	88.932	-1.754
2300	63.996	478.695	420.599	84.743	-1.559
2400	63.995	481.419	423.077	80.649	-1.383
2500	64.017	484.031	425.463	76.658	-1.223
2600	64.059	486.543	427.765	72.783	-1.077
2700	64.120	488.962	429.987	69.024	-0.944
2800	64.198	491.295	432.135	65.385	-0.822
2900	64.289	493.549	434.214	61.864	-0.712
3000	64.393	495.730	436.228	58.462	-0.612
3100	64.507	497.844	438.182	55.187	-0.528
3200	64.630	499.894	440.079	52.042	-0.459
3300	64.760	501.884	441.921	49.024	-0.402
3400	64.895	503.820	443.714	46.130	-0.356
3500	65.034	505.703	445.458	43.363	-0.311
3600	65.175	507.537	447.157	40.731	-0.260
3700	65.317	509.324	448.813	38.232	-0.212
3800	65.458	511.068	450.429	35.869	-0.167
3900	65.599	512.770	452.005	33.643	-0.124
4000	65.738	514.433	453.545	31.556	-0.085
4100	65.873	516.058	455.050	29.609	-0.047
4200	66.005	517.647	456.522	27.802	-0.012
4300	66.133	519.201	457.962	26.133	0.021
4400	66.257	520.723	459.371	24.605	0.053
4500	66.375	522.214	460.751	23.218	0.083
4600	66.487	523.674	462.103	21.974	0.111
4700	66.594	525.105	463.428	20.870	0.138
4800	66.695	526.508	464.728	19.905	0.164
4900	66.790	527.884	466.003	19.076	0.188
5000	66.879	529.234	467.254	18.377	0.212
5100	66.962	530.559	468.482	17.799	0.235
5200	67.038	531.860	469.688	17.338	0.258
5300	67.109	533.138	470.874	16.984	0.281
5400	67.173	534.393	472.038	16.736	0.304
5500	67.232	535.626	473.183	16.592	0.327
5600	67.284	536.838	474.309	16.550	0.350
5700	67.331	538.029	475.417	16.609	0.373
5800	67.373	539.201	476.506	16.768	0.396
5900	67.409	540.353	477.579	17.027	0.419
6000	67.440	541.486	478.634	17.386	0.442

Δ<sub>f</sub>H°(0 K) = [257.38 ± 41.8] kJ·mol<sup>-1</sup>  
 Δ<sub>f</sub>H°(298.15 K) = [257.73 ± 41.8] kJ·mol<sup>-1</sup>

S°(298.15 K) = [339.290 ± 8.4] J·K<sup>-1</sup>·mol<sup>-1</sup>

Electronic Levels and Quantum Weights	
ε <sub>r</sub> , cm <sup>-1</sup>	g <sub>r</sub>
0	[1]
[243.1]	[3]
[669.6]	[5]
[1225.2]	[7]
[1873.0]	[9]
[11471.3]	[11]
[12590.8]	[13]
[12630.3]	[15]
[13201.3]	[17]
[13741.5]	[19]

Vibrational Frequencies and Degeneracies	
v, cm <sup>-1</sup>	
[200](1)	
[50](2)	
[200](1)	

σ = [2]

Point Group: [D<sub>2h</sub>]  
 Bond Distance: Mo-I = [2.66] Å  
 Bond Angle: I-Mo-I = [180]<sup>o</sup>  
 Rotational Constant: B<sub>0</sub> = [0.009387] cm<sup>-1</sup>

Enthalpy of Formation

The adopted value of Δ<sub>f</sub>H° at 298.15 K is that estimated by Brewer.<sup>1</sup> The estimated value is consistent with the low volatility of solid molybdenum in iodine vapor reported by Schafer *et al.*<sup>2</sup> Brewer has given no weight to the equilibrium data reported by Allen and Yost<sup>3</sup> for the formation of MoI<sub>2</sub>(g) from Mo(s) and I<sub>2</sub>(g) since the product formed may have been MoO<sub>3</sub>, rather than the diiodide.<sup>2</sup> Brewer's estimated value is given as Δ<sub>f</sub>H°(298.15 K) = 31000 ± 5000 K. The assigned uncertainty (± 10 kcal·mol<sup>-1</sup>) is determined from the product 5000 × R which has been rounded to the nearest kcal·mol<sup>-1</sup>. The value of Δ<sub>f</sub>H°(0 K) combined with JANAF data for Mo(g) and I<sub>2</sub>(g) gives Δ<sub>f</sub>H°(0 K) = 147 ± 11 kcal·mol<sup>-1</sup> and an average Mo-I bond energy of Δ<sub>b</sub>H°(0 K) = 73.4 ± 5.5 kcal·mol<sup>-1</sup>.

Heat Capacity and Entropy

The bond length and vibrational frequencies are values estimated by Brewer.<sup>1</sup> A linear structure has been predicted for MoI<sub>2</sub> by Drake and Rosenblatt.<sup>5</sup> The electronic contribution is taken to be the same as that for the free gaseous Mo<sup>2+</sup> ion, as estimated by Brewer.<sup>1</sup> The levels listed by Rico<sup>6</sup> below 1374 cm<sup>-1</sup> are used in the calculations.

Our heat capacity and enthalpy values up to 3000 K are in agreement with those determined by Brewer.<sup>1</sup> However, his entropies and free energy functions differ from our values by about 1 cal·K<sup>-1</sup>·mol<sup>-1</sup> at all temperatures over the range 298-3000 K. We believe that his results are erroneous due to the use of an incorrect value for the molecular weight of MoI<sub>2</sub>. We reproduce his entropies and free energy functions if we use a molecular weight of 476.65 which corresponds to MoI<sub>3</sub>.

References

- L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley personal communication, September 20, 1978, preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria.
- H. Schafer, T. Grofe, and M. Trenkel, *J. Solid State Chem.* **8**, 14 (1973).
- T. L. Allen and D. M. Yost, *J. Chem. Phys.* **22**, 855 (1954).
- JANAF Thermochemical Tables: Mo(g), 3-31-78, I(g), 6-30-74.
- M. C. Drake and G. M. Rosenblatt, Paper 388, The Electrochemical Society, Atlanta, Georgia, (October 1977).
- F. R. Rico, *An. Real Soc. Espan. Fis. Quim., Ser. A* **61**, 103 (1965).

PREVIOUS: September 1978 (1 atm)

CURRENT: September 1978 (1 bar)

Molybdenum Iodide (MoI<sub>2</sub>)

I<sub>2</sub>Mo<sub>2</sub>(g)

IDEAL GAS

Iodine Oxide (IOI)

$\Delta_f H^\circ(0 \text{ K}) = 348 \pm 25 \text{ kJ mol}^{-1}$   
 $S^\circ(298.15 \text{ K}) = [308.1 \pm 4] \text{ J K}^{-1} \text{ mol}^{-1}$

Electronic Level and Quantum Weight state	$\epsilon_n, \text{cm}^{-1}$	$g_n$
X'A	0.0	1

Vibrational Frequencies and Degeneracies

$\nu, \text{cm}^{-1}$
[475](1)
[100](1)
[525](1)

Point Group:  $C_{2v}$   
 Bond Distance: I-O = [2.0]Å  
 Bond Angle I-O-I = [115]°  
 Product of the Moments of Inertia:  $I_A I_B I_C = 42498.6720 \times 10^{-117} \text{ g}^3 \text{ cm}^6$

$\sigma = 2$

Enthalpy of Formation

For the series XO(g) [where X = F, Cl, Br, I], there are only reliable experimental data for ClOCl(g) and  $D_0^0(\text{ClO})$  and  $\Delta_f H^\circ(\text{ClOCl}_g)$  are reasonable, we adopt the ratio of the numbers (1.52) to apply for a similar relationship between IO(g) and IOI(g). The ratio for the corresponding bromine oxides is approximately 1.6.

Heat Capacity and Entropy

The structure of this molecule is estimated to be bent with a I-O-I angle of [115]° and a bond length of [2.0]Å in analogy with the corresponding fluorine, chlorine, and bromine oxide molecules.<sup>1</sup> The principal moments of inertia in  $\text{g cm}^2$  are  $I_A = 2.8860 \times 10^{-39}$ ,  $I_B = 119.9153 \times 10^{-39}$ , and  $I_C = 122.8013 \times 10^{-39}$ .

The vibrational frequencies are estimated from known frequencies of FOF(g), ClOCl(g), and BrOBr(g)<sup>1</sup> and expected trends in this halogen oxide family.

References

<sup>1</sup>NIST-JANAF Thermochemical Tables. FOF(g), September 1995; ClOCl(g), March 1996, BrOBr(g), (March 1996).

Iodine Oxide (IOI)

$M_r = 269.80834$

Enthalpy Reference Temperature =  $T_r = 298.15 \text{ K}$   
 $S^\circ = -[G^\circ - H^\circ(T_r)]/T$

Standard State Pressure =  $p^\circ = 0.1 \text{ MPa}$   
 $\Delta_f H^\circ$

T/K	$C_p^\circ$	$S^\circ$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta G^\circ$	$\log K_r$
0	.000	INFINITE			124.000	INFINITE
50	37.610	230.650	-11.291	124.000	124.000	
100	40.943	250.463	-9.318	124.056	117.968	-123.241
150	44.704	275.070	-7.192	124.303	112.182	-38.598
200	47.472	288.246	-4.898	124.204	106.886	-37.221
250	50.053	299.131	-2.456	123.522	101.928	-26.621
298.15	51.874	308.111	.000	120.522	97.207	-20.510
300	51.933	308.432	.096	119.485	92.832	-16.264
400	54.269	323.727	5.418	119.453	92.667	-16.135
500	55.547	335.988	10.915	101.652	84.560	-11.042
600	56.302	346.187	16.511	57.423	84.562	-8.834
700	56.780	354.905	21.166	57.684	89.965	-7.832
800	57.100	362.509	27.161	57.945	95.323	-7.113
900	57.324	369.248	33.583	58.193	100.648	-6.572
1000	57.487	375.297	39.324	58.422	105.941	-6.149
1100	57.608	380.782	45.079	58.630	111.209	-5.809
1200	57.701	385.799	50.845	58.815	116.458	-5.530
1300	57.774	390.420	56.619	58.973	121.691	-5.297
1400	57.832	394.704	62.399	59.100	126.912	-5.099
1500	57.879	398.695	68.185	59.187	132.125	-4.930
1600	57.918	402.432	73.975	59.204	137.333	-4.782
1700	57.950	405.944	79.768	59.115	142.541	-4.653
1800	57.977	409.258	85.565	58.953	147.752	-4.540
1900	58.000	412.393	91.364	58.712	152.970	-4.439
2000	58.019	415.368	97.165	58.391	158.199	-4.349
2100	58.036	418.200	102.967	57.993	163.444	-4.269
2200	58.051	420.900	108.772	57.523	168.706	-4.196
2300	58.064	423.481	114.578	56.986	173.989	-4.131
2400	58.075	425.952	120.384	56.386	179.294	-4.072
2500	58.085	428.323	126.192	55.765	184.624	-4.018
2600	58.094	430.601	132.001	55.100	189.980	-3.969
2700	58.101	432.794	137.811	55.100	195.361	-3.925
2800	58.108	434.907	143.622	54.414	200.769	-3.884
2900	58.115	436.946	149.433	53.720	206.203	-3.842
3000	58.120	438.916	155.245	53.027	211.660	-3.812
3100	58.125	440.822	161.057	52.347	217.142	-3.781
3200	58.130	442.668	166.870	51.688	222.646	-3.752
3300	58.134	444.457	172.683	51.058	228.171	-3.725
3400	58.138	446.192	178.496	50.462	233.715	-3.699
3500	58.142	447.877	184.311	49.907	239.277	-3.676
3600	58.145	449.515	190.125	49.397	244.854	-3.654
3700	58.148	451.109	195.940	48.934	250.445	-3.634
3800	58.151	452.659	201.754	48.522	256.048	-3.615
3900	58.153	454.170	207.570	48.161	261.663	-3.597
4000	58.156	455.642	213.385	47.853	267.288	-3.580
4100	58.158	457.078	219.201	47.598	272.915	-3.564
4200	58.160	458.480	225.017	47.395	278.550	-3.549
4300	58.162	459.848	230.833	47.245	284.190	-3.534
4400	58.164	461.185	236.649	47.147	289.833	-3.521
4500	58.165	462.493	242.466	47.099	295.477	-3.508
4600	58.167	463.771	248.282	47.099	301.122	-3.495
4700	58.168	465.022	254.099	47.147	306.766	-3.483
4800	58.170	466.247	259.916	47.241	312.410	-3.472
4900	58.171	467.446	265.733	47.378	318.050	-3.461
5000	58.172	468.621	271.550	47.558	323.688	-3.451
5100	58.173	469.773	277.367	47.777	329.321	-3.440
5200	58.174	470.903	283.185	48.035	334.950	-3.431
5300	58.175	472.011	289.002	48.329	340.572	-3.421
5400	58.176	473.098	294.820	48.658	346.189	-3.412
5500	58.177	474.166	300.638	49.018	351.799	-3.403
5600	58.178	475.214	306.455	49.409	357.403	-3.394
5700	58.179	476.244	312.273	306.455	363.000	-3.386
5800	58.180	477.256	318.091	50.274	368.588	-3.378
5900	58.181	478.250	323.909	50.744	374.168	-3.370
6000	58.181	479.228	329.727	51.237	379.740	-3.362
				51.751	385.304	-3.354

PREVIOUS:

CURRENT: March 1996 (1 bar)

Iodine Oxide (IOI)

I<sub>2</sub>O(g)



Iodine Oxide (IO)

IDEAL GAS

$M_r = 269.80834$  Iodine Oxide (IO)

$I_2O_1(g)$

$S^\circ(298.15\text{ K}) = [330.6 \pm 4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$

$\Delta_f H^\circ(0\text{ K}) = [110.5 \pm 40] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [106.7 \pm 40] \text{ kJ}\cdot\text{mol}^{-1}$

Electronic Level and Quantum Weight state	$\epsilon_e, \text{cm}^{-1}$	g.
[ $^1A_1$ ]	0.0	[3]

Vibrational Frequencies and Degeneracies

$\nu, \text{cm}^{-1}$
[750](1)
[1000](1)
[1700](1)

Point Group,  $C_2$   
 Bond Distances: I-O = [1.9]Å ; I-I = [3.0]Å  
 Bond Angle: I-O-I = [125]°  
 Product of the Moments of Inertia:  $I_A I_B I_C = 67538.6868 \times 10^{-117} \text{ g}^3\cdot\text{cm}^6$   
 $\sigma = 1$

Enthalpy of Formation

For the four halogen oxide species,  $XXO(g)$  where  $X = \text{F, Cl, Br, I}$ , there are no experimental data related to the enthalpy of formation. Thus the enthalpy of formation is estimated based on assumption that the X-X bond in  $XXO(g)$  is  $0.6 D_0^0(X_2)$ . This leads to a  $\Delta_f H^\circ(\text{IO}, 0\text{ K}) = 110.5 \text{ kJ}\cdot\text{mol}^{-1}$ .

Heat Capacity and Entropy

The structure of this molecule is estimated to be bent with a I-I-O angle of [125]° and bond distances  $r(\text{I-I}) = [3.0]\text{Å}$  and  $r(\text{I-O}) = [1.9]\text{Å}$ . This structure is estimated in analogy with the corresponding chlorine and bromine molecules. The vibrational frequencies are estimated from the known frequencies of  $\text{ClIO}$  and  $\text{BrBrO}$ . The principal moments of inertia in  $\text{g}\cdot\text{cm}^2$  are:  $I_A = 5.1010 \times 10^{-39}$ ,  $I_B = 112.5438 \times 10^{-39}$ , and  $I_C = 117.6448 \times 10^{-39}$ .

References

<sup>1</sup>NIST-JANAF Thermochemical Tables:  $\text{ClIO}(g)$ ; March 1996;  $\text{BrBrO}(g)$ ; (March 1996).

T/K	Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$		log $K_f$
	$C_p^\circ$	$S^\circ - [C_p^\circ - F(T_r)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	
0	0.000	INFINITE	-13.691	110.500	INFINITE
50	39.124	247.843	-11.942	110.572	103.624
100	45.462	271.774	-7.870	109.826	-108.255
150	47.981	286.239	-7.438	109.104	30.629
200	49.683	310.283	-5.015	108.286	31.534
250	51.153	321.531	-2.493	107.452	-22.087
298.15	52.359	330.647	.000	106.652	-16.431
300	52.401	330.971	.097	106.621	-12.838
400	54.230	346.316	5.435	88.835	-12.723
500	55.386	358.551	10.970	44.594	-8.189
600	56.127	368.719	16.499	63.601	-6.315
700	56.620	377.411	22.138	65.083	-5.537
800	56.961	384.995	27.818	66.708	-4.978
900	57.205	391.719	33.527	68.451	-4.556
1000	57.384	397.756	38.499	70.300	-4.227
1100	57.520	403.232	42.631	72.252	-3.962
1200	57.625	408.241	46.054	74.304	-3.744
1300	57.707	412.857	48.775	76.454	-3.562
1400	57.773	417.136	50.863	78.700	-3.408
1500	57.827	421.124	52.373	81.041	-3.275
1600	57.872	424.857	53.400	83.475	-3.160
1700	57.909	428.367	54.054	85.900	-3.060
1800	57.940	431.678	54.333	88.316	-2.971
1900	57.966	434.811	54.232	90.722	-2.892
2000	57.989	437.785	53.863	93.118	-2.822
2100	58.008	440.615	53.243	95.505	-2.759
2200	58.025	443.314	52.384	97.882	-2.703
2300	58.040	445.894	51.303	100.250	-2.652
2400	58.053	448.364	49.920	102.618	-2.607
2500	58.065	450.734	48.256	104.985	-2.567
2600	58.075	453.012	46.320	107.352	-2.528
2700	58.084	455.204	44.124	109.719	-2.494
2800	58.092	457.316	41.673	112.086	-2.463
2900	58.100	459.355	39.076	114.453	-2.434
3000	58.106	461.325	36.325	116.820	-2.408
3100	58.112	463.230	33.430	119.187	-2.384
3200	58.118	465.075	30.393	121.554	-2.362
3300	58.123	466.865	27.216	123.921	-2.342
3400	58.127	468.599	23.900	126.288	-2.323
3500	58.131	470.284	20.455	128.655	-2.306
3600	58.135	471.921	16.890	131.022	-2.290
3700	58.139	473.514	13.215	133.389	-2.275
3800	58.142	475.065	9.540	135.756	-2.261
3900	58.145	476.575	5.865	138.123	-2.248
4000	58.148	478.047	2.190	140.490	-2.236
4100	58.150	479.483	-1.485	142.857	-2.224
4200	58.153	480.884	-4.170	145.224	-2.213
4300	58.155	482.253	-6.855	147.591	-2.203
4400	58.157	483.590	-9.540	149.958	-2.193
4500	58.159	484.897	-12.225	152.325	-2.183
4600	58.161	486.175	-14.910	154.692	-2.174
4700	58.163	487.426	-17.595	157.059	-2.166
4800	58.164	488.650	-20.280	159.426	-2.157
4900	58.166	489.850	-22.965	161.793	-2.149
5000	58.167	491.025	-25.650	164.160	-2.142
5100	58.168	492.177	-28.335	166.527	-2.134
5200	58.170	493.306	-31.020	168.894	-2.127
5300	58.171	494.414	-33.705	171.261	-2.120
5400	58.172	495.502	-36.390	173.628	-2.114
5500	58.173	496.569	-39.075	175.995	-2.107
5600	58.174	497.617	-41.760	178.362	-2.101
5700	58.175	498.647	-44.445	180.729	-2.094
5800	58.176	499.659	-47.130	183.096	-2.088
5900	58.177	500.653	-49.815	185.463	-2.082
6000	58.178	501.631	-52.500	187.830	-2.077

PREVIOUS:

CURRENT March 1996 (1 bar)

Iodine Oxide (IO)

$I_2O_1(g)$

Lead Iodide (PbI<sub>2</sub>)

## CRYSTAL

M<sub>r</sub> = 461.0090Lead Iodide (PbI<sub>2</sub>)I<sub>2</sub>Pb<sub>1</sub>(cr)

$S^{\circ}(298.15 \text{ K}) = 174.836 \pm 0.21 \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = 683 \pm 2 \text{ K}$   
 $\Delta_{\text{fus}}H^{\circ}(10 \text{ K}) = -174.817 \pm 0.42 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{fus}}H^{\circ}(298.15 \text{ K}) = -175.393 \pm 0.42 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{fus}}H^{\circ} = 23.430 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$

## Enthalpy of Formation

Koref and Braune<sup>1</sup> determined  $\Delta_{\text{f}}H^{\circ}(\text{PbI}_2, \text{cr}, 298.15 \text{ K}) = -41.850 \text{ kcal}\cdot\text{mol}^{-1}$  by enthalpy of solution calorimetry 3rd law analyses of emf data at 298.15 K reported by Gerke<sup>2</sup> and Cann and Taylor<sup>3</sup> for the reaction  $\text{Pb}(\text{cr}) + \text{I}_2(\text{cr}) = \text{PbI}_2(\text{cr})$  lead to  $\Delta_{\text{f}}H^{\circ}(\text{PbI}_2, \text{cr}, 298.15 \text{ K}) = -41.923$  and  $-41.925 \text{ kcal}\cdot\text{mol}^{-1}$ , respectively.  $\Delta_{\text{f}}H^{\circ}(\text{PbI}_2, \text{cr}, 298.15 \text{ K}) = -41.92 \pm 0.10 \text{ kcal}\cdot\text{mol}^{-1}$  is adopted.

## Heat Capacity and Entropy

McBride<sup>4</sup> measured the low temperature heat capacity (4.52–291.00 K) of PbI<sub>2</sub>. Enthalpies have been measured by Ehrhardt<sup>5</sup> (448–776 K), Magnus<sup>6</sup> (373–523 K), and Linsley<sup>7</sup> (323–877 K). The enthalpy data of Linsley<sup>7</sup> is subjected to a curve fitting procedure subject to the constraint that it join smoothly in the region of 298.15 K with the enthalpy derived from the heat capacity data of McBride<sup>4</sup>.  $S^{\circ}(10 \text{ K}) = 0.662 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  is adopted from McBride.<sup>4</sup> The data of Linsley<sup>7</sup> did not indicate any transitions other than the solid liquid transition at 683 K.

## Fusion Data

Germann and Metz<sup>8</sup> van Klooster and Stearns<sup>9</sup> and Popovkin, Odin, and Novoselova<sup>10</sup> determined  $T_{\text{fus}} = 685 \pm 1 \text{ K}$  Blanc and Petit<sup>11</sup> found  $T_{\text{fus}} = 680 \text{ K}$ . Sumarokova and Modestova<sup>12</sup> found PbI<sub>2</sub> to exist in two crystalline forms with the  $\alpha$ -B transition at 645 K. On a DTA cooling curve, Popovkin *et al.*<sup>10</sup> observed a peak at 656 K which they attribute to the B- $\alpha$  transition. Modestova and Sumarokova<sup>13</sup> observed the B form to melt at 669 K. Ehrhardt<sup>5</sup> drop calorimetry data and his interpretation of the enthalpy increase at 648 K as indicating the melting points are consistent with the existence of a B-phase. The observation by Novoselova *et al.*<sup>14</sup> that only the  $\alpha$  form crystallizes on cooling melts of the PbI<sub>2</sub> rich region of the PbI<sub>2</sub>-PbSe system is consistent with the interpretation that the reference state for Ehrhardt's work is  $\alpha$ -PbI<sub>2</sub>. The enthalpy measurements by Linsley<sup>7</sup> led to a reported value of  $T_{\text{fus}} = 683 \text{ K}$ . This value is adopted.

From a plot of Ehrhardt's enthalpy data,  $\Delta_{\text{fus}}H^{\circ} = 5.43 \text{ kcal}\cdot\text{mol}^{-1}$  at 683 K is obtained. Kelley<sup>15</sup> derived 5.57, 5.67, and 5.80 kcal·mol<sup>-1</sup> from phase diagram information and also gives 6.01 kcal·mol<sup>-1</sup>. Another analysis<sup>16</sup> has resulted in  $\Delta_{\text{fus}}H^{\circ} = 5.20 \text{ kcal}\cdot\text{mol}^{-1}$ . Blanc and Petit's<sup>11</sup> value of 3.87 kcal·mol<sup>-1</sup> is too low. The enthalpy data of Linsley<sup>7</sup> was analyzed to yield  $\Delta_{\text{fus}}H^{\circ} = 5.6 \text{ kcal}\cdot\text{mol}^{-1}$ .  $\Delta_{\text{fus}}H^{\circ} = 5.6 \pm 0.2 \text{ kcal}\cdot\text{mol}^{-1}$  is adopted.

## Sublimation Data

$\Delta_{\text{sub}}H^{\circ}(298.15 \text{ K})$  is calculated from the difference between the adopted values for  $\Delta_{\text{f}}H^{\circ}(298.15 \text{ K})$  of the gas and crystal. Refer to PbI<sub>2</sub>(g) table.

## References

- <sup>1</sup>F. Koref and H. Braune, *Z. Elektrochem.*, **18**, 818 (1912).
- <sup>2</sup>R. H. Gerke, *J. Amer. Chem. Soc.*, **44**, 1684 (1922).
- <sup>3</sup>J. Y. Cann and A. C. Taylor, *J. Amer. Chem. Soc.*, **59**, 1987 (1937).
- <sup>4</sup>J. J. McBride, Ph.D. Dissertation, University of Michigan, (1955).
- <sup>5</sup>O. Ehrhardt, *Wied. Ann.*, **24**, 215 (1885).
- <sup>6</sup>A. Magnus, *Ann. Physik*, **31**, 597 (1910).
- <sup>7</sup>C. W. Linsley, Ph.D. Dissertation, North Texas State University, (1970).
- <sup>8</sup>F. E. Germann and C. F. Metz, *J. Phys. Chem.*, **35**, 1944 (1931).
- <sup>9</sup>H. S. van Klooster and E. E. Stearns, *J. Amer. Chem. Soc.*, **55**, 4121 (1933).
- <sup>10</sup>B. A. Popovkin, I. N. Odin, A. V. Novoselova, *Vestn. Mosk. Univ.*, **Khim.**, **12**, 316 (1971).
- <sup>11</sup>M. Blanc and G. Petit, *Compt. rend.*, **248**, 1305 (1959).
- <sup>12</sup>T. N. Sumarokova, and T. Modestova, *Zhur. Neorg. Khim.*, **1**, 2027 (1956).
- <sup>13</sup>T. Modestova and T. N. Sumarokova, *Zhur. Neorg. Khim.*, **3**, 1655 (1958).
- <sup>14</sup>A. V. Novoselova, I. N. Odin, and B. A. Popovkin, *Isv. Akad. Nauk SSSR*, Neorg. Mater. **2**, 1397 (1966).
- <sup>15</sup>K. K. Kelley, U. S. Bur. Mines Bull. 393, 166 pp. (1936).
- <sup>16</sup>K. K. Kelley, U. S. Bur. Mines Bull. 584, 232 pp. (1960).
- <sup>17</sup>U. S. Nat. Bur. Stand. Circ. 500, 1268 pp. (1952).

T/K	C <sub>p</sub> <sup>a</sup>	S <sup>b</sup> - [G <sup>c</sup> - H <sup>c</sup> (T)]/T	H <sup>c</sup> - H <sup>c</sup> (T)	$\Delta_{\text{f}}H^{\circ}$	Standard State Pressure = $p^{\circ} = 0.1 \text{ MPa}$	log K <sub>r</sub>
0	0	INFINITE	-19.501	-174.817	-174.817	INFINITE
100	69.789	93.717	-14.839	-174.972	-174.562	91.182
200	75.396	144.332	-7.506	-175.096	-174.116	45.474
298.15	71.573	174.836	0	-175.393	-173.577	30.410
300	71.613	175.316	0.144	-175.400	-173.566	30.221
400	78.856	197.846	7.978	-191.933	-172.328	22.504
500	80.391	215.574	15.925	-234.996	-163.287	17.059
600	83.713	230.498	24.116	-233.448	-149.087	12.979
683.000	87.780	241.591	31.226	---	CRYSTAL $\leftarrow$ LIQUID	---
700	88.743	243.761	32.726	-236.428	-134.371	10.027
800	95.102	256.015	41.910	-234.040	-119.947	7.832
900	102.428	267.637	51.784	-230.941	-105.864	6.144
1000	110.064	278.821	62.406	-227.076	-92.166	4.814

PREVIOUS: March 1962

CURRENT: December 1973

Lead Iodide (PbI<sub>2</sub>)I<sub>2</sub>Pb<sub>1</sub>(cr)

$I_2Pb_2(l)$

$M_r = 461.0090$  Lead Iodide ( $PbI_2$ )

LIQUID

Lead Iodide ( $PbI_2$ )

$S^\circ(298.15\text{ K}) = [198.902] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = 683 \pm 2 \text{ K}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [-157.679] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{vap}} H^\circ = 23.430 \pm 0.8 \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**

$\Delta_f H^\circ(PbI_2, l, 298.15\text{ K})$  is calculated from  $\Delta_f H^\circ(PbI_2, cr, 298.15\text{ K})$  by adding  $\Delta_{\text{fus}} H^\circ$  and the difference in the enthalpy,  $H^\circ(683\text{ K}) - H^\circ(298.15\text{ K})$ , between the crystal and the liquid.  
 $\Delta_f H^\circ(l)$  can also be obtained from a 2nd and 3rd law analysis of emf data for the cell reaction  $Pb(l) + I_2(g) = PbI_2(l)$  as reported by Murgulescu *et al.*<sup>1</sup> in the form of an equation covering a range of 723 to 923 K. The enthalpy changes for the reaction are  $\Delta_f H^\circ(298.15\text{ K}) = 57.65 \pm 0.18 \text{ kcal}\cdot\text{mol}^{-1}$  (2nd law) and  $-52.74 \pm 1.08 \text{ kcal}\cdot\text{mol}^{-1}$  (3rd law) with a drift of  $5.8 \pm 0.2 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . With auxiliary data  $\Delta_f H^\circ(Pb, l, 298.15\text{ K}) = 1.025 \text{ kcal}\cdot\text{mol}^{-1}$  and  $\Delta_f H^\circ(I_2, g, 298.15\text{ K}) = 14.924 \text{ kcal}\cdot\text{mol}^{-1}$ ,<sup>2</sup>  $\Delta_f H^\circ(PbI_2, l, 298.15\text{ K}) = 41.70 \text{ kcal}\cdot\text{mol}^{-1}$  and  $-36.79 \text{ kcal}\cdot\text{mol}^{-1}$  from the 2nd and 3rd law calculations, respectively.

**Heat Capacity and Entropy**

The heat capacity is assumed to be constant at  $25.95 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  from 460 to 2000 K and is based on a linear least squares fit of the liquid range enthalpy measurements (683–877 K) of Linsey.<sup>4</sup> The enthalpy measurements of Ehrhardt<sup>3</sup> for the liquid range covered a smaller temperature region (687–776 K) and are considered less reliable. A least squares fit of the Ehrhardt data<sup>3</sup> leads to a heat capacity value of  $32.5 \text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$ . A glass transition is assumed at 460 K below which the heat capacity is that of the crystal.  
 $S^\circ(PbI_2, l, 298.15\text{ K})$  is calculated in a manner analogous to that used for the enthalpy of formation.

**Vaporization Data**

$T_{\text{vap}} = 1105\text{ K}$  is calculated as the temperature at which the fugacity is 1 atm for the reaction  $PbI_2(cr) = PbI_2(g)$ .  $\Delta_{\text{vap}} H^\circ = 28.34 \text{ kcal}\cdot\text{mol}^{-1}$  is calculated as the difference between  $\Delta_f H^\circ$  at  $T_{\text{vap}}$  for the gas and the liquid.

**References**

- <sup>1</sup>I. G. Murgulescu, S. Sternberg, and M. Terzi, *Electrochim. Acta* **12**, 1121 (1967).
- <sup>2</sup>JANAF Thermochemical Tables: Pb(0), 3–31–62,  $I_2(g)$ , 9–30–61.
- <sup>3</sup>O. Ehrhardt, *Wied. Ann.* **24**, 215 (1885).
- <sup>4</sup>C. W. Linsey, Ph.D. Dissertation, North Texas State University, (1970).

Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$				
$T/K$	$C_p^\circ$	$S^\circ - [G^\circ - H^\circ(T)]/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta G^\circ$	$\log K_f$
0						
100						
200						
298.15	77.571	198.902	198.902	0.	-157.679	28.564
300	77.613	199.382	198.904	0.144	-157.686	28.393
400	78.856	221.912	201.967	7.978	-174.219	21.448
460.000	79.592	232.980	205.306	12.730	GLASS $\leftarrow$ LIQUID	
460.000	108.575	232.980	205.306	12.730	TRANSITION	
500	108.575	242.033	207.887	17.073	-216.134	16.470
600	108.575	261.829	215.278	36.942	-211.920	12.741
683.000	108.575	275.896	221.808	38.788	CRYSTAL $\leftarrow$ LIQUID	
700	108.575	278.565	223.154	49.643	-212.652	10.071
800	108.575	293.064	231.007	60.503	-208.591	8.105
900	108.575	305.852	238.627	71.360	-204.509	6.606
1000	108.575	317.291	245.931	82.218	-200.408	5.431
1100	108.575	327.640	252.896	93.075	-196.290	4.489
1200	108.575	337.087	259.524	103.933	-192.159	3.720
1300	108.575	345.778	265.829	114.790	-188.028	3.083
1400	108.575	353.824	271.831	125.648	-183.920	2.549
1500	108.575	361.315	277.550		-179.855	2.097

PREVIOUS: March 1962

CURRENT: December 1973

Lead Iodide ( $PbI_2$ )

$I_2Pb_2(l)$

Lead Iodide (PbI<sub>2</sub>)

CRYSTAL-LIQUID

Lead Iodide (PbI<sub>2</sub>)

I<sub>2</sub>Pb<sub>1</sub>(cr,l)

0 to 683 K crystal  
above 683 K liquid

Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature - T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa	
	C <sup>*</sup>	S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	ΔG°
0	0	0	0	0
100	69.789	93.717	-19.501	-174.817
200	75.396	144.332	-148.339	-174.862
298.15	77.573	174.836	-7.506	-174.116
300	77.613	174.838	0	-175.393
400	78.856	197.846	0.144	-175.400
500	80.391	215.574	7.978	-172.328
600	83.713	230.498	15.925	-234.996
683.000	87.780	241.591	24.116	-233.448
683.000	108.575	275.896	31.226	-149.087
700	108.575	278.565	56.502	12.979
800	108.575	293.064	197.848	CRYSTAL <--> LIQUID TRANSITION
900	108.575	305.852	208.864	-212.652
1000	108.575	317.291	218.944	-134.959
1100	108.575	327.640	228.217	-208.591
1200	108.575	337.087	236.792	-124.137
1300	108.575	345.778	244.762	-204.509
1400	108.575	353.824	252.203	-113.825
1500	108.575	361.315	259.178	-200.408
			265.740	89.074
				99.932
				106.200
				-94.524
				4.489
				192.150
				110.786
				131.647
				188.028
				76.150
				132.504
				183.920
				-68.323
				-179.833
				-60.208
				10.071
				8.105
				6.606
				5.431
				4.489
				3.720
				2.063
				2.549
				2.097

PREVIOUS

CURRENT: December 1973

Lead Iodide (PbI<sub>2</sub>)

I<sub>2</sub>Pb<sub>1</sub>(cr,l)

IDEAL GAS

Lead Iodide (PbI<sub>2</sub>)

M<sub>r</sub> = 461.0090 Lead Iodide (PbI<sub>2</sub>)

I<sub>2</sub>PbI(g)

S°(298.15 K) = [359.552 ± 8.4] J·K<sup>-1</sup>·mol<sup>-1</sup> Δ<sub>f</sub>H°(298.15 K) = -3.18 ± 4.2 kJ·mol<sup>-1</sup> Δ<sub>f</sub>H°(0 K) = -1.16 ± 4.2 kJ·mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies

$\nu_1$ , cm <sup>-1</sup>	[100](1)
	[40](1)
	[160](1)

Ground State Quantum Weight: [1] σ = 2

Point Group: C<sub>2v</sub>

Bond Distance: Pb-I = 2.79 ± 0.02 Å

Bond Angle: Br-Pb-Br = [95]°

Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [2.948087 × 10<sup>-111</sup>] g<sup>3</sup>·cm<sup>6</sup>

Enthalpy of Formation

The adopted value of Δ<sub>f</sub>H°(298.15 K) = 0.76 ± 1.0 kcal·mol<sup>-1</sup> is the average of results from 3rd law analyses of two sets<sup>1,2</sup> of sublimation data and one set<sup>3</sup> of vaporization data. Auxiliary data Δ<sub>f</sub>H°(PbI<sub>2</sub>, cr, 298.15 K) = -41.92 kcal·mol<sup>-1</sup> and Δ<sub>f</sub>H°(PbI<sub>2</sub>, l, 298.15 K) = -37.686 kcal·mol<sup>-1</sup> are used in the calculations. The adopted enthalpy of formation for PbI<sub>2</sub>(g) yields an atomization energy of Δ<sub>at</sub>H°(0 K) = 4.29 eV for the process PbI<sub>2</sub>(g) = Pb(g) + 2 I(g).

Source	Reaction	Data Points	T/K	Δ <sub>f</sub> H°, kcal·mol <sup>-1</sup>	Drift	Δ <sub>f</sub> H°(PbI <sub>2</sub> , g, 298.15 K)
Niva <i>et al.</i> <sup>1</sup>	A	7	579-650	39.77 ± 0.37	41.54 ± 0.16	2.9 ± 0.60
Duncan and Thomas <sup>2</sup>	A	13	563-613	39.44 ± 0.40	40.24 ± 0.09	1.4 ± 0.7
Jellinek and Rudat <sup>3</sup>	B	4	923-1073	35.19 ± 0.52	37.49 ± 0.32	2.3 ± 0.6

\*Reactions: (A) PbI<sub>2</sub>(cr) = PbI<sub>2</sub>(g) (B) PbI<sub>2</sub>(l) = PbI<sub>2</sub>(g)

Heat Capacity and Entropy

Molecular dimensions are those given by Sutton.<sup>5</sup> Vibrational frequencies are estimated by comparison with the corresponding values for HgI<sub>2</sub>(g) and with the lead dihalide series.<sup>6</sup> The electronic ground state is assumed to be A<sub>1</sub> based on analogy with PbCl<sub>2</sub>(g).<sup>6</sup> The principal moments of inertia are: I<sub>A</sub> = 67.3005 × 10<sup>-39</sup>, I<sub>B</sub> = 178.3336 × 10<sup>-39</sup> and I<sub>C</sub> = 245.6341 × 10<sup>-39</sup> g·cm<sup>2</sup>.

References

- <sup>1</sup>K. Niva, M. Sato, and M. Yosiyama, *J. Chem. Soc. Japan* 60, 918 (1939).
- <sup>2</sup>J. F. Duncan and F. G. Thomas, *J. Chem. Soc.* 1964, 360 (1964).
- <sup>3</sup>K. Jellinek and A. Rudat, *Z. physik. Chem.* 143, 55 (1929).
- <sup>4</sup>JANAF Thermochemical Tables: PbI<sub>2</sub>(cr), 12-31-73; PbI<sub>2</sub>(l), 12-31-73; HgI<sub>2</sub>(g), 3-31-62; PbF<sub>2</sub>(g), 12-31-73; PbBr<sub>2</sub>(g), 12-31-73.
- <sup>5</sup>L. E. Sutton, Ed., "Tables of Interatomic Distances and Configuration in Molecules and Ions." The Chemical Society, London, (1958).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - [G° - H°(T)]/T	H° - H°(T <sub>r</sub> )	Δ <sub>f</sub> G°	
0	0	INFINITE	-11.736	1.161	INFINITE
100	53.807	298.094	410.195	0.870	10.007
200	56.934	336.667	364.806	-1.005	-38.492
250	57.375	349.424	360.499	-2.078	-47.741
298.15	57.615	359.552	359.552	-3.180	-56.437
300	57.622	359.908	359.553	-3.224	-56.767
350	57.773	368.803	360.255	-4.504	-65.393
400	57.872	376.524	361.817	-6.181	-73.681
450	57.940	383.345	363.837	-8.778	-80.012
500	57.989	389.452	366.099	-11.677	-85.262
600	58.054	400.031	370.899	-17.479	-94.082
700	58.092	408.983	375.717	-23.287	-101.836
800	58.118	416.742	380.371	-29.097	-107.856
900	58.135	423.588	384.800	-34.910	-112.882
1000	58.148	429.714	388.990	-40.724	-117.259
1100	58.157	435.257	392.948	-46.539	-121.119
1200	58.164	440.317	396.688	-52.355	-124.512
1300	58.169	444.973	400.216	-58.172	-127.484
1400	58.174	449.284	403.578	-63.989	-130.070
1500	58.177	453.298	406.760	-69.807	-132.325
1600	58.180	457.053	409.787	-75.625	-134.228
1700	58.182	460.580	412.672	-81.443	-135.836
1800	58.184	463.906	415.427	-87.261	-137.206
1900	58.186	467.052	418.062	-93.080	-138.386
2000	58.188	470.036	420.587	-98.898	-139.414
2100	58.190	472.875	423.010	-104.717	-140.325
2200	58.191	475.582	425.338	-110.536	-141.145
2300	58.191	478.169	427.580	-116.355	-141.873
2400	58.192	480.645	429.739	-122.174	-142.519
2500	58.192	483.021	431.823	-127.993	-143.083
2600	58.193	485.303	433.837	-133.813	-143.565
2700	58.194	487.499	435.784	-139.632	-144.000
2800	58.194	489.616	437.669	-145.451	-144.395
2900	58.195	491.636	439.495	-151.271	-144.752
3000	58.195	493.631	441.267	-157.090	-145.081
3100	58.195	495.539	442.987	-162.910	-145.386
3200	58.196	497.338	444.659	-168.729	-145.666
3300	58.196	499.171	446.284	-174.548	-145.924
3400	58.196	500.915	447.865	-180.368	-146.165
3500	58.197	502.602	449.405	-186.188	-146.388
3600	58.197	504.241	450.906	-192.008	-146.595
3700	58.197	505.836	452.369	-197.827	-146.786
3800	58.197	507.388	453.796	-203.647	-146.962
3900	58.197	508.899	455.190	-209.467	-147.124
4000	58.198	510.373	456.551	-215.287	-147.273
4100	58.198	511.810	457.882	-221.106	-147.411
4200	58.198	513.212	459.192	-226.926	-147.539
4300	58.198	514.582	460.455	-232.746	-147.657
4400	58.198	515.920	461.670	-238.566	-147.766
4500	58.198	517.228	462.820	-244.386	-147.866
4600	58.198	518.507	463.914	-250.205	-147.957
4700	58.198	519.758	465.235	-256.025	-148.040
4800	58.199	520.984	466.433	-261.845	-148.115
4900	58.199	522.184	467.558	-267.665	-148.182
5000	58.199	523.359	468.662	-273.485	-148.241
5100	58.199	524.512	469.746	-279.305	-148.292
5200	58.199	525.642	470.810	-285.125	-148.336
5300	58.199	526.751	471.855	-290.945	-148.374
5400	58.199	527.838	472.882	-296.764	-148.407
5500	58.199	528.906	473.891	-302.584	-148.435
5600	58.199	529.955	474.883	-308.404	-148.459
5700	58.199	530.985	475.858	-314.224	-148.479
5800	58.199	531.997	476.817	-320.044	-148.495
5900	58.199	532.992	477.761	-325.864	-148.508
6000	58.199	533.970	478.690	-331.684	-148.518

PREVIOUS December 1973 (1 atm) CURRENT December 1973 (1 bar)

Lead Iodide (PbI<sub>2</sub>)

I<sub>2</sub>PbI(g)

Diiodosilylene (SiI<sub>2</sub>)

Diiodosilylene (SiI<sub>2</sub>)

I<sub>2</sub>Si<sub>1</sub>(g)

S°(298.15 K) = [320.972 ± 4.2] J K<sup>-1</sup> mol<sup>-1</sup>  
 Δ<sub>f</sub>H°(0 K) = 95.09 ± 8.4 kJ mol<sup>-1</sup>  
 Δ<sub>f</sub>H°(298.15 K) = 92.47 ± 8.4 kJ mol<sup>-1</sup>

Electronic Levels and Quantum Weights	g <sub>e</sub>
State	
[ <sup>1</sup> A <sub>1</sub> ]	0
[ <sup>1</sup> B <sub>1</sub> ]	[20000]
Vibrational Frequencies and Degeneracies	
ν, cm <sup>-1</sup>	
[350](1)	
[90](1)	
[350](1)	

Point Group [C<sub>2v</sub>]  
 Bond Distance Si-I = [2.44] Å  
 Bond Angle I-Si-I = [113]°  
 Product of the Moments of Inertia I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [2.419819 × 10<sup>-112</sup>] g<sup>3</sup>cm<sup>6</sup>

Enthalpy of Formation

An equilibrium system involving SiI<sub>2</sub>(g) has been studied by Schafer *et al.*<sup>1</sup> and Wolf and Herbst.<sup>2</sup> They both used a flow technique in an argon atmosphere. A 2nd and 3rd law analysis of their results (reported only in equation form) is summarized below. As in the case of SiCl<sub>2</sub>(g) and SiBr<sub>2</sub>(g), there is acceptable agreement between the 3rd law results of these two studies. Using the mean Δ<sub>f</sub>H°(298.15 K), we calculate and adopt Δ<sub>f</sub>H°(SiI<sub>2</sub>, g, 298.15 K) = 92.47 ± 8.4 kJ mol<sup>-1</sup>. This corresponds to Δ<sub>f</sub>H° = 135.2 kcal mol<sup>-1</sup> and an average bond energy of 67.6 kcal mol<sup>-1</sup>. In comparison, the average bond energy of SiI<sub>4</sub>(g) is 58.6 kcal mol<sup>-1</sup>. This implies that the average bond energy is 15% stronger in SiI<sub>2</sub> than in SiI<sub>4</sub>.

Source	Reaction	T/K	Δ <sub>f</sub> H°(298.15 K), kcal mol <sup>-1</sup>	Drift	Δ <sub>f</sub> H°(g, 298.15 K)*
1	SiI <sub>2</sub> (g) = SiI <sub>2</sub> (g) + 2I(g)	1361-1526	98.92	1.46	23.60
2	Si(cr) + I <sub>2</sub> (g) = SiI <sub>2</sub> (g)	1300-1470	3.21	1.38	20.60
4	SiI <sub>2</sub> (g) + Si(cr) = 2SiI <sub>2</sub> (g)	1173-1373	83.90	-12.42	20.84

\*Based on 3rd law Δ<sub>f</sub>H°(298.15 K) value and auxiliary data<sup>3</sup>.

Uchimura *et al.*<sup>4</sup> also studied SiI<sub>2</sub>(g). An analysis of their equilibrium data yields Δ<sub>f</sub>H°(SiI<sub>2</sub>, g, 298.15 K) = 20.84 kcal mol<sup>-1</sup>, which is in good agreement with our adopted value. However, because of the large drift (-12.42 cal K<sup>-1</sup> mol<sup>-1</sup>), no weight was given to this study.

Heat Capacity and Entropy

The Si-I bond distance is assumed to be the same as in SiH<sub>2</sub>.<sup>3</sup> The bond angle is estimated to be 113° based on the trend observed in SiF<sub>2</sub>, SiCl<sub>2</sub>, and SiBr<sub>2</sub>. C<sub>2v</sub> symmetry is also assumed to be consistent with the other three silicon dihalides. The principal moments of inertia are I<sub>A</sub> = 7.6158 × 10<sup>-39</sup>, I<sub>B</sub> = 174.4841 × 10<sup>-39</sup>, and I<sub>C</sub> = 182.0999 × 10<sup>-39</sup> g cm<sup>2</sup>.

The vibrational frequencies are estimated based on trends observed in the SiX<sub>2</sub> and SiH<sub>2</sub>X<sub>2</sub> species, where X = F, Cl, Br, and I.<sup>3</sup> As suggested by SiF<sub>2</sub> and SiCl<sub>2</sub>, an electronic excited state is included at 20000 cm<sup>-1</sup>.

References

- <sup>1</sup>H. Schafer, H. Bruderrick, and B. Morcher, *Z. anorg. allg. Chem.* **352**, 122 (1967).
- <sup>2</sup>E. Wolf and C. Herbst, *Z. Chem.* **7**, 34 (1967).
- <sup>3</sup>JANAF Thermochemical Tables, Si(g), 3-31-67, I(g), 6-30-74, SiH<sub>2</sub>F<sub>2</sub>(g) and SiI<sub>4</sub>(g), 6-30-76, SiBr<sub>2</sub>(g), SiH<sub>2</sub>X<sub>2</sub>(g), X = Cl, Br, and I,<sup>3</sup> 12-31-76; SiF<sub>2</sub>(g), SiCl<sub>2</sub>(g), and SiBr<sub>2</sub>(g), 12-31-77.
- <sup>4</sup>K. Uchimura, T. Takuma, M. Yuzumi, and T. Kunugi, *Denki Kagaku* **35**, 876 (1967).

T/K	C <sub>p</sub> <sup>o</sup>	S°	-[C <sub>p</sub> <sup>o</sup> - H°(T <sub>o</sub> )]/T	H° - H°(T <sub>o</sub> )	Δ <sub>f</sub> H°	Standard State Pressure = p° = 0.1 MPa	log K <sub>1</sub>
0	0	0	INFINITE	INFINITE	95.090	95.090	INFINITE
100	43.279	266.948	367.003	-10.006	95.561	95.561	95.348
200	51.344	299.763	325.883	-5.224	94.231	94.231	14.572
250	53.375	311.456	321.865	-2.602	93.375	93.375	-9.620
298.15	54.624	320.972	320.972	0	92.466	92.466	-6.484
300	54.663	321.310	320.973	0.101	92.430	92.430	-6.384
350	55.512	329.804	321.641	2.857	91.339	91.339	-4.097
400	56.096	337.257	323.137	5.648	74.217	74.217	-18.952
450	56.512	343.889	325.081	8.464	71.875	71.875	-14.14
500	56.817	349.860	327.266	11.297	29.392	29.392	-0.990
600	57.226	360.259	331.923	17.001	28.966	28.966	-0.482
700	57.478	369.100	336.618	22.737	28.486	28.486	-0.172
800	57.644	376.787	341.170	28.494	27.955	27.955	-0.136
900	57.759	383.584	345.512	34.265	27.373	27.373	0.340
1000	57.842	389.674	349.629	40.045	26.741	26.741	0.497
1100	57.904	395.190	353.524	45.832	26.057	26.057	-13.110
1200	57.951	400.220	357.209	51.628	25.318	25.318	-16.638
1300	57.988	404.870	360.699	57.422	24.519	24.519	-20.103
1400	58.017	409.169	364.010	63.222	23.650	23.650	-23.503
1500	58.040	413.172	367.155	69.025	22.701	22.701	-26.838
1600	58.060	416.919	370.150	74.830	21.663	21.663	-30.108
1700	58.076	420.439	373.005	80.637	20.551	20.551	-33.322
1800	58.090	423.759	375.734	86.445	30.563	30.563	-36.495
1900	58.102	426.900	378.345	92.255	-31.743	-31.743	-39.624
2000	58.113	429.881	380.848	98.066	-32.892	-32.892	-42.713
2100	58.124	432.716	383.251	103.878	-34.008	-34.008	-45.762
2200	58.135	435.420	385.561	109.690	-35.185	-35.185	-48.775
2300	58.147	438.005	387.785	115.503	-36.316	-36.316	-51.751
2400	58.160	440.480	389.930	121.320	-37.400	-37.400	-54.688
2500	58.176	442.854	392.000	127.137	-38.497	-38.497	-57.579
2600	58.195	445.136	394.000	132.955	-39.599	-39.599	-60.436
2700	58.218	447.333	395.935	138.776	-40.706	-40.706	-63.266
2800	58.245	449.451	397.808	144.599	-41.818	-41.818	-66.069
2900	58.274	451.495	399.625	150.425	-42.935	-42.935	-68.846
3000	58.317	453.472	401.387	156.255	-44.058	-44.058	-71.597
3100	58.363	455.385	403.098	162.089	-45.186	-45.186	-74.324
3200	58.416	457.238	404.761	167.928	-46.318	-46.318	-77.027
3300	58.477	459.037	406.379	173.772	-47.454	-47.454	-79.706
3400	58.546	460.784	407.953	179.623	-48.594	-48.594	-82.361
3500	58.624	462.482	409.487	185.482	-49.738	-49.738	-85.000
3600	58.710	464.134	410.982	191.349	-50.886	-50.886	-87.623
3700	58.805	465.744	412.440	197.224	-52.038	-52.038	-90.232
3800	58.909	467.314	413.864	203.110	-53.194	-53.194	-92.827
3900	59.022	468.846	415.254	209.006	-54.354	-54.354	-95.408
4000	59.143	470.341	416.613	214.915	-55.518	-55.518	-97.975
4100	59.273	471.803	417.941	220.833	-56.686	-56.686	-100.528
4200	59.411	473.233	419.241	226.769	-57.858	-57.858	-103.067
4300	59.557	474.633	420.513	232.718	-59.034	-59.034	-105.592
4400	59.710	476.004	421.758	238.681	-60.214	-60.214	-108.104
4500	59.870	477.348	422.979	244.660	-61.400	-61.400	-110.603
4600	60.036	478.665	424.175	250.655	-62.592	-62.592	-113.090
4700	60.208	479.958	425.348	256.667	-63.790	-63.790	-115.564
4800	60.385	481.228	426.499	262.697	-65.000	-65.000	-118.035
4900	60.567	482.475	427.629	268.745	-66.222	-66.222	-120.500
5000	60.753	483.700	428.738	274.811	-67.456	-67.456	-122.960
5100	60.943	484.905	429.827	280.896	-68.702	-68.702	-125.415
5200	61.135	486.090	430.898	286.999	-70.000	-70.000	-127.865
5300	61.330	487.257	431.950	293.123	-71.358	-71.358	-130.310
5400	61.526	488.405	432.985	299.265	-72.776	-72.776	-132.750
5500	61.723	489.536	434.003	305.428	-74.254	-74.254	-135.185
5600	61.920	490.650	435.005	311.610	-75.792	-75.792	-137.615
5700	62.118	491.747	435.991	317.812	-77.390	-77.390	-140.040
5800	62.315	492.829	436.961	324.034	-79.048	-79.048	-142.460
5900	62.511	493.896	437.917	330.275	-80.766	-80.766	-144.875
6000	62.705	494.948	438.859	336.536	-82.544	-82.544	-147.285

PREVIOUS December 1977 (1 atm)

CURRENT December 1977 (1 bar)

Diiodosilylene (SiI<sub>2</sub>)

I<sub>2</sub>Si<sub>1</sub>(g)

I<sub>2</sub>Sr<sub>1</sub>(cr)

M<sub>r</sub> = 341.4290 Strontium Iodide (SrI<sub>2</sub>)

CRYSTAL

Strontium Iodide (SrI<sub>2</sub>)

Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa			
T/K	C <sub>p</sub> <sup>o</sup> / J·K <sup>-1</sup> ·mol <sup>-1</sup>	S° - (G° - H°(T <sub>r</sub> ))/T / J·K <sup>-1</sup> ·mol <sup>-1</sup>	H° - H°(T <sub>r</sub> ) / kJ·mol <sup>-1</sup>	Δ <sub>f</sub> H° / kJ·mol <sup>-1</sup>	log K <sub>r</sub>
0	0	INFINITE	-18.919	-560.645	INFINITE
100	67.404	78.914	-14.725	-559.988	292.508
200	75.019	128.568	-7.519	-558.896	145.969
298.15	77.948	159.120	0	-557.702	97.707
300	78.032	159.603	0.144	-557.678	97.100
400	80.751	182.421	8.083	-557.928	72.579
500	83.513	200.737	16.296	-620.739	57.035
600	86.274	216.207	24.785	-618.933	46.262
700	88.994	229.710	33.548	-616.972	38.375
800	91.755	241.776	42.587	-614.852	32.830
811.000	92.048	243.031	43.598	---	---
900	94.492	252.741	51.899	-613.204	28.373
1000	97.236	262.839	61.486	-610.453	24.822
1100	99.971	272.234	71.346	-615.344	21.912
1200	102.717	281.051	81.480	-612.989	19.482
1300	105.493	289.382	91.891	-610.380	17.433
1400	108.240	297.301	102.578	-607.527	15.685
1500	110.960	304.861	113.538	-604.440	14.178

Δ<sub>f</sub>H°(0 K) = -560.65 ± 2.1 kJ·mol<sup>-1</sup>  
 Δ<sub>f</sub>H°(298.15 K) = -561.49 ± 2.1 kJ·mol<sup>-1</sup>  
 Δ<sub>sub</sub>H° = 19.665 ± 0.38 kJ·mol<sup>-1</sup>  
 Δ<sub>sub</sub>H°(298.15 K) = 286.604 kJ·mol<sup>-1</sup>

**Enthalpy of Formation**  
 Ehrlich *et al.*<sup>1</sup> derived Δ<sub>f</sub>H°(SrI<sub>2</sub>, cr, 298.15 K) = -133.8 ± 0.4 kcal mol<sup>-1</sup> from enthalpy of solution measurements of Sr(cr) and SrI<sub>2</sub>(cr) in 0.1 N HI. An auxiliary HI enthalpy of solution value, -13.22 kcal·mol<sup>-1</sup>, calculated from data in reference<sup>2</sup> was used in the derivation. This auxiliary value will be changed by incorporation of the accepted CODATA key value of Δ<sub>f</sub>H°(I, aq, std. state) = -13.60 kcal·mol<sup>-1</sup> in the Δ<sub>f</sub>H°(HI, aq, 298.15 K) table so that the above derived enthalpy of formation of SrI<sub>2</sub>(cr) will be approximately -134.3 kcal·mol<sup>-1</sup>. Combining Δ<sub>f</sub>H°(Sr<sup>2+</sup>, aq, std. state, 298.15 K) = -130.45 kcal mol<sup>-1</sup> selected by Parker<sup>3</sup> with the CODATA value for I(aq, std. state)<sup>4</sup> gives Δ<sub>f</sub>H°(SrI<sub>2</sub>, aq, std. state, 298.15 K) = 157.65 kcal·mol<sup>-1</sup>. Further combination with the enthalpy of solution, 23.43 kcal·mol<sup>-1</sup> gives Δ<sub>f</sub>H°(SrI<sub>2</sub>, cr, 298.15 K) = -134.22 kcal·mol<sup>-1</sup>. This enthalpy of solution value is based solely on the work of Ehrlich *et al.*<sup>5</sup> To be consistent with the selection of the enthalpies of formation of BaI<sub>2</sub>(cr) and CaI<sub>2</sub>(cr), we adopt Δ<sub>f</sub>H°(SrI<sub>2</sub>, cr, 298.15 K) = -134.2 ± 0.5 kcal·mol<sup>-1</sup> calculated via the combination of aqueous ions.

**Heat Capacity and Entropy**  
 C<sub>p</sub><sup>o</sup>(13.9–300.9 K) has been measured by Paukov *et al.*<sup>1</sup> and smoothed values have been published. Starting values of entropy and enthalpy, S°(14 K) and H°(14 K) H°(0 K), were not given. Our T<sup>3</sup> extrapolation leads to S°(8 K) = 0.148 cal·K<sup>-1</sup>·mol<sup>-1</sup> and H°(8 K) H°(0 K) = 0.891 cal·K<sup>-1</sup>·mol<sup>-1</sup>, which, when combined with our C<sub>p</sub><sup>o</sup> extrapolation from 14 K to 8 K and with the Paukov *et al.*<sup>1</sup> data, gives S°(298.15 K) = 38.03 cal·K<sup>-1</sup>·mol<sup>-1</sup> and H°(298.15 K) H°(0 K) = 4522 cal·K<sup>-1</sup>·mol<sup>-1</sup>. Paukov *et al.*<sup>1</sup> gave 37.42 ± 0.06 cal·K<sup>-1</sup>·mol<sup>-1</sup> and 4156 ± 7 kcal·mol<sup>-1</sup> for the entropy and enthalpy at 298.15 K. In as much as our integration of their data gives S°(298.15 K) = 37.26 cal·K<sup>-1</sup>·mol<sup>-1</sup> it appears unlikely that their published value for S°(298.15 K) is correct.

The low temperature heat capacity joins smoothly with a linear extrapolation from C<sub>p</sub><sup>o</sup> = 18.45 at 270 K to C<sub>p</sub><sup>o</sup> = 22.0 at the adopted T<sub>m</sub> of 811 K. The linearly extrapolated heat capacity at 298 K is 0.6% higher than the published smoothed value<sup>7</sup> Dworkin and Bredig<sup>8</sup> determined the heat capacity of the crystal near the melting point to be 22.9 ± 5%. The graphically selected C<sub>p</sub><sup>o</sup>(811 K) = 22.0 is within the experimental error and gives H°(811 K) H°(298.15 K) = 10.42 kcal·mol<sup>-1</sup> in agreement with Dworkin and Bredig's measured value of 10.4 kcal·mol<sup>-1</sup>.

**Fusion Data**  
 Emmons and Loeffelholz<sup>9</sup> determined Δ<sub>sub</sub>H° = 4.580 kcal·mol<sup>-1</sup> (±5%) and T<sub>sub</sub> = 802 K by high temperature cryoscopy, in good agreement with the drop calorimetry Δ<sub>sub</sub>H° = 4.70 kcal·mol<sup>-1</sup> (±2%) and T<sub>sub</sub> = 811 K by Dworkin and Bredig.<sup>8</sup> Hutchison<sup>10</sup> found T<sub>sub</sub> = 793 K, noting that his melting point data were only approximate.  
 Because drop calorimetry is a more direct measure of the enthalpy of melting, we adopt Δ<sub>sub</sub>H° = 4.70 ± 0.09 kcal·mol<sup>-1</sup> at T<sub>sub</sub> = 811 ± 10 K.

**Sublimation Data**  
 Δ<sub>sub</sub>H°(298.15 K) is derived as the difference between the enthalpies of formation of the ideal gas and the crystal state at 298.15 K.

**References**  
<sup>1</sup>P. Ehrlich, K. Peik, and E. Koch, *Z. anorg. allg. Chem.* **324**, 113 (1963).  
<sup>2</sup>U. S. Nat. Bur. Stand. Circ. 500, 1268 pp.(1952).  
<sup>3</sup>J. D. Cox, ICSU CODATA Task Group on Key Values for Thermodynamics, *J. Chem. Thermodyn.* **4**, 331 (1972).  
<sup>4</sup>V. B. Parker, U. S. Nat. Bur. Stand. Report 10074, 164 (1969).  
<sup>5</sup>U. S. Nat. Bur. Stand. Tech. Note 270-6, 119 pp. (1971).  
<sup>6</sup>V. B. Parker, U. S. Nat. Bur. Stand., personal communication, (May 1974).  
<sup>7</sup>I. E. Paukov, F. S. Vrublevskaia, Russ. *J. Phys. Chem.* **47**, 1226 (1973).  
<sup>8</sup>A. S. Dworkin and M. A. Bredig, *J. Phys. Chem.* **67**, 697 (1963).  
<sup>9</sup>H. H. Emmons and B. Loeffelholz, *Wiss. Z. Hochsch. Chem. Leuna Merseburg* **6**, 261 (1964).  
<sup>10</sup>J. F. Hutchison, *U. S. At. Energy Comm. IS-T-50*, (1965).

PREVIOUS:

CURRENT: June 1974

Strontium Iodide (SrI<sub>2</sub>)

I<sub>2</sub>Sr<sub>1</sub>(cr)

Strontium Iodide (SrI <sub>2</sub> )		Strontium Iodide (SrI <sub>2</sub> )		I <sub>2</sub> Sr <sub>2</sub> (l)		
LIQUID		LIQUID		I <sub>2</sub> Sr <sub>2</sub> (l)		
$M_r = 341.4290$		$M_r = 341.4290$		$M_r = 341.4290$		
$\Delta_f H^\circ(298.15 \text{ K}) = [-548.748] \text{ kJ} \cdot \text{mol}^{-1}$		$\Delta_f H^\circ(298.15 \text{ K}) = [-548.748] \text{ kJ} \cdot \text{mol}^{-1}$		$\Delta_f H^\circ(298.15 \text{ K}) = [-548.748] \text{ kJ} \cdot \text{mol}^{-1}$		
$\Delta_{\text{vap}} H^\circ = 19.665 \pm 0.38 \text{ kJ} \cdot \text{mol}^{-1}$		$\Delta_{\text{vap}} H^\circ = 19.665 \pm 0.38 \text{ kJ} \cdot \text{mol}^{-1}$		$\Delta_{\text{vap}} H^\circ = 19.665 \pm 0.38 \text{ kJ} \cdot \text{mol}^{-1}$		
$S^\circ(298.15 \text{ K}) = [172.440] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$		$S^\circ(298.15 \text{ K}) = [172.440] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$		$S^\circ(298.15 \text{ K}) = [172.440] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$		
$T_{\text{fus}} = 811 \pm 10 \text{ K}$		$T_{\text{fus}} = 811 \pm 10 \text{ K}$		$T_{\text{fus}} = 811 \pm 10 \text{ K}$		
Enthalpy of Formation		Enthalpy of Formation		Enthalpy of Formation		
$\Delta_f H^\circ(\text{SrI}_2, \text{l}, 298.15 \text{ K})$ is calculated from $\Delta_f H^\circ(\text{SrI}_2, \text{cr}, 298.15 \text{ K})$ by adding the enthalpy of fusion, $\Delta_{\text{fus}} H^\circ$ , and the difference in enthalpy, $H^\circ(811 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and the liquid.		$\Delta_f H^\circ(\text{SrI}_2, \text{l}, 298.15 \text{ K})$ is calculated from $\Delta_f H^\circ(\text{SrI}_2, \text{cr}, 298.15 \text{ K})$ by adding the enthalpy of fusion, $\Delta_{\text{fus}} H^\circ$ , and the difference in enthalpy, $H^\circ(811 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and the liquid.		$\Delta_f H^\circ(\text{SrI}_2, \text{l}, 298.15 \text{ K})$ is calculated from $\Delta_f H^\circ(\text{SrI}_2, \text{cr}, 298.15 \text{ K})$ by adding the enthalpy of fusion, $\Delta_{\text{fus}} H^\circ$ , and the difference in enthalpy, $H^\circ(811 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and the liquid.		
Heat Capacity and Entropy		Heat Capacity and Entropy		Heat Capacity and Entropy		
The liquid heat capacity near the melting point, $26.3 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ , was determined by Dworkin and Bredig <sup>1</sup> from drop calorimeter measurements. This value is adopted and assumed constant over a 500–2600 K range. A glass transition is assumed at 500 K below which the heat capacity is that of the crystal.		The liquid heat capacity near the melting point, $26.3 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ , was determined by Dworkin and Bredig <sup>1</sup> from drop calorimeter measurements. This value is adopted and assumed constant over a 500–2600 K range. A glass transition is assumed at 500 K below which the heat capacity is that of the crystal.		The liquid heat capacity near the melting point, $26.3 \text{ cal} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$ , was determined by Dworkin and Bredig <sup>1</sup> from drop calorimeter measurements. This value is adopted and assumed constant over a 500–2600 K range. A glass transition is assumed at 500 K below which the heat capacity is that of the crystal.		
$S^\circ(\text{SrI}_2, \text{l}, 298.15 \text{ K})$ is calculated in a manner similar to that used for the enthalpy of formation.		$S^\circ(\text{SrI}_2, \text{l}, 298.15 \text{ K})$ is calculated in a manner similar to that used for the enthalpy of formation.		$S^\circ(\text{SrI}_2, \text{l}, 298.15 \text{ K})$ is calculated in a manner similar to that used for the enthalpy of formation.		
Vaporization Data		Vaporization Data		Vaporization Data		
The temperature at which the fugacity is 1 atm for the reaction $\text{SrI}_2(\text{l}) = \text{SrI}_2(\text{g})$ is 2181 K, the adopted $T_{\text{vap}}$ . Peterson and Hutchison have extrapolated Knudsen effusion cell measurements in the 1061–1308 K range to obtain a normal boiling point of 2046 K.		The temperature at which the fugacity is 1 atm for the reaction $\text{SrI}_2(\text{l}) = \text{SrI}_2(\text{g})$ is 2181 K, the adopted $T_{\text{vap}}$ . Peterson and Hutchison have extrapolated Knudsen effusion cell measurements in the 1061–1308 K range to obtain a normal boiling point of 2046 K.		The temperature at which the fugacity is 1 atm for the reaction $\text{SrI}_2(\text{l}) = \text{SrI}_2(\text{g})$ is 2181 K, the adopted $T_{\text{vap}}$ . Peterson and Hutchison have extrapolated Knudsen effusion cell measurements in the 1061–1308 K range to obtain a normal boiling point of 2046 K.		
$\Delta_{\text{vap}} H^\circ = 45.35 \text{ kcal} \cdot \text{mol}^{-1}$ is the calculated difference between the enthalpies of formation of the ideal gas and the liquid at $T_{\text{vap}}$ . Refer to the ideal gas table for details.		$\Delta_{\text{vap}} H^\circ = 45.35 \text{ kcal} \cdot \text{mol}^{-1}$ is the calculated difference between the enthalpies of formation of the ideal gas and the liquid at $T_{\text{vap}}$ . Refer to the ideal gas table for details.		$\Delta_{\text{vap}} H^\circ = 45.35 \text{ kcal} \cdot \text{mol}^{-1}$ is the calculated difference between the enthalpies of formation of the ideal gas and the liquid at $T_{\text{vap}}$ . Refer to the ideal gas table for details.		
References		References		References		
<sup>1</sup> A. S. Dworkin and M. A. Bredig, <i>J. Phys. Chem.</i> <b>67</b> , 697 (1963).		<sup>1</sup> A. S. Dworkin and M. A. Bredig, <i>J. Phys. Chem.</i> <b>67</b> , 697 (1963).		<sup>1</sup> A. S. Dworkin and M. A. Bredig, <i>J. Phys. Chem.</i> <b>67</b> , 697 (1963).		
<sup>2</sup> D. T. Peterson and J. F. Hutchison, <i>J. Chem. Eng. Data</i> <b>15</b> , 320 (1970).		<sup>2</sup> D. T. Peterson and J. F. Hutchison, <i>J. Chem. Eng. Data</i> <b>15</b> , 320 (1970).		<sup>2</sup> D. T. Peterson and J. F. Hutchison, <i>J. Chem. Eng. Data</i> <b>15</b> , 320 (1970).		
T/K	$C_p^\circ$	$S^\circ - (C_p^\circ - H^\circ(T))/T$	$H^\circ - H^\circ(T)$	$\Delta_f H^\circ$	$\Delta G^\circ$	log K <sub>f</sub>
0						
100						
200						
298.15	77.948	172.440	172.440	0.	-548.748	96.170
300	78.032	172.923	172.442	0.144	-548.754	95.577
400	80.751	195.741	175.534	8.083	-565.183	71.610
499.990	83.513	214.055	181.464	16.295	-548.373	
499.990	110.039	214.055	181.464	16.295	-548.373	
500	110.039	214.057	181.465	16.296	-540.057	56.419
600	110.039	234.120	188.620	27.300	-603.674	45.869
700	110.039	251.082	196.362	38.304	-599.471	38.386
800	110.039	265.776	204.141	49.308	-595.386	32.813
811.000	110.039	267.279	204.987	50.518	-595.386	
900	110.039	278.737	211.724	60.312	-592.047	28.503
1000	110.039	290.330	219.015	71.316	-587.878	25.078
1100	110.039	300.818	225.982	82.320	-581.170	22.279
1200	110.039	310.393	232.623	93.323	-578.401	19.844
1300	110.039	319.201	238.949	104.327	-585.199	17.979
1400	110.039	327.356	244.976	115.331	-582.028	16.304
1500	110.039	334.948	250.724	126.335	-578.898	14.860
1600	110.039	342.049	256.212	137.339	-575.818	13.603
1700	110.039	348.720	261.460	148.343	-572.710	12.464
1800	110.039	355.010	266.484	159.347	-569.599	11.257
1900	110.039	360.960	271.301	170.351	-566.487	10.184
2000	110.039	366.604	275.926	181.355	-563.375	9.225
2100	110.039	371.973	280.373	192.359	-560.263	8.362
2200	110.039	377.092	284.654	203.363	-557.151	7.584
2300	110.039	381.983	288.780	214.367	-554.039	6.877
2400	110.039	386.666	292.762	225.370	-550.927	6.234
2500	110.039	391.158	296.609	236.374	-547.815	5.646
2600	110.039	395.474	300.329	247.378	-544.703	5.107

PREVIOUS:

CURRENT June 1974

Strontium Iodide (SrI<sub>2</sub>)I<sub>2</sub>Sr<sub>2</sub>(l)



Strontium Iodide (SrI<sub>2</sub>)

M<sub>r</sub> = 341.4290 Strontium Iodide (SrI<sub>2</sub>)

CRYSTAL-LIQUID

0 to 811 K crystal  
above 811 K liquid

Refer to the individual tables for details.

I<sub>2</sub>SrI(cr,l)

Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa			
T/K	C <sub>p</sub> <sup>o</sup> J·K <sup>-1</sup> ·mol <sup>-1</sup>	S° - [C <sub>p</sub> <sup>o</sup> - R ln(T <sub>r</sub> /T)]/T J·K <sup>-1</sup> ·mol <sup>-1</sup>	H° - H°(T <sub>r</sub> ) kJ·mol <sup>-1</sup>	Δ <sub>f</sub> G° kJ·mol <sup>-1</sup>	log K <sub>f</sub>
0	0	0	INFINITE	-560.645	INFINITE
100	67.404	78.914	276.165	-561.001	292.508
200	75.019	128.568	166.164	-561.216	145.969
298.15	77.948	159.120	159.120	-561.493	97.707
300	78.032	159.603	159.122	0.144	97.100
400	80.751	182.421	162.214	8.083	72.579
500	83.513	200.737	168.145	16.296	57.055
600	86.274	216.207	174.898	24.785	46.262
700	88.994	229.710	181.784	33.446	38.575
800	91.755	241.776	188.542	42.587	32.830
811.000	92.048	243.031	189.272	43.598	—
811.000	110.039	267.279	189.272	63.263	—
900	110.039	278.737	197.563	73.057	28.503
1000	110.039	290.330	206.270	84.061	25.078
1100	110.039	300.818	214.396	95.064	22.279
1200	110.039	310.393	222.003	106.068	19.944
1300	110.039	319.201	229.145	117.072	17.979
1400	110.039	327.356	235.873	128.076	16.304
1500	110.039	334.948	242.227	139.080	14.860
1600	110.039	342.049	248.247	150.084	13.603
1700	110.039	348.720	253.963	161.088	12.464
1800	110.039	355.010	259.403	172.092	11.257
1900	110.039	360.960	264.593	183.096	10.184
2000	110.039	366.604	269.554	194.100	9.225
2100	110.039	371.973	274.304	205.104	8.362
2200	110.039	377.092	278.861	216.108	7.584
2300	110.039	381.983	283.239	227.111	6.877
2400	110.039	386.666	287.432	238.115	6.234
2500	110.039	391.158	291.511	249.119	5.646
2600	110.039	395.474	295.427	260.123	5.107

CRYSTAL <---> LIQUID  
TRANSITION

PREVIOUS:

CURRENT: June 1974

Strontium Iodide (SrI<sub>2</sub>)

I<sub>2</sub>SrI(cr,l)

Strontium Iodide (SrI<sub>2</sub>)

## IDEAL GAS

M<sub>r</sub> = 341.4290 Strontium Iodide (SrI<sub>2</sub>)I<sub>2</sub>Sr<sub>1</sub>(g)

$$298.15 \text{ K} = [339.554 \pm 8.4] \text{ J K}^{-1} \text{ mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = -274.89 \pm 6.3 \text{ kJ mol}^{-1}$$

$$\Delta_f H^\circ(0 \text{ K}) = -271.66 \pm 6.3 \text{ kJ mol}^{-1}$$

## Vibrational Frequencies and Degeneracies

$\nu$ , cm <sup>-1</sup>
(111)(1)
(31)(2)
(219)(1)

Ground State Quantum Weight: [1]

Point Group: D<sub>2h</sub>

Bond Distance: Sr-I = 3.03 ± 0.03 Å

Bond Angle: I-Sr-I = [180]°

Rotational Constant: B<sub>0</sub> = 0.007234 cm<sup>-1</sup>

σ = 2

## Enthalpy of Formation

Peterson and Hutchison<sup>12</sup> used a weight loss Knudsen effusion technique to observe vapor pressures of the liquid at 20 temperatures ranging from 1061 to 1308 K. Our 2nd and 3rd law analyses of these data give  $\Delta_{\text{vap}}H^\circ(298.15 \text{ K}) = 65.72 \pm 1.48 \text{ kcal mol}^{-1}$  and  $\Delta_{\text{vap}}H^\circ(298.15 \text{ K}) = 65.48 \pm 0.68 \text{ kcal mol}^{-1}$  with a drift of  $-0.2 \pm 1.2 \text{ cal K}^{-1} \text{ mol}^{-1}$ . We adopt  $\Delta_{\text{vap}}H^\circ(298.15 \text{ K}) = 65.5 \pm 0.7 \text{ kcal mol}^{-1}$  and combine this with the adopted enthalpy of formation of the liquid to obtain  $\Delta_f H^\circ(\text{SrI}_2, \text{g}, 298.15 \text{ K}) = -65.7 \pm 1.5 \text{ kcal mol}^{-1}$ .

## Heat Capacity and Entropy

The bond distance, as determined from an electron diffraction study, is taken from Akishin *et al.*<sup>13</sup> who also judged that the bond angle was  $180^\circ \pm 10^\circ$ . We have assumed a linear structure.

An analysis of the trend of the ratio of the stretching force constants,  $k(\text{monohalide})/k(\text{dihalide})$ , has indicated that  $k(\text{SrI})/k(\text{SrI}_2) = 1$  is a reasonable approximation.<sup>4</sup> The bending force constant is taken as 0.01 times the stretching force constant. These approximations have been used by Brewer *et al.*<sup>5</sup> Our vibrational frequencies calculated from the force constants, using  $k$  for SrI calculated from the ground state vibrational frequency given by Rosen,<sup>6</sup> are in exact agreement with those calculated by Brewer *et al.*,<sup>5</sup> which are adopted. Other estimates of  $\nu_1$ ,  $\nu_2$ , and  $\nu_3$  are 111, 49, and 220.<sup>7</sup>

We assign an uncertainty of  $\pm 2 \text{ cal K}^{-1} \text{ mol}^{-1}$  to the entropy to allow for error in bond angle and vibrational frequency estimates.

## References

- J. F. Hutchison, U. S. At Energy Comm. IS-T-50, (1965).
- D. T. Peterson and J. F. Hutchison, J. Chem. Eng. Data 15, 320 (1970).
- P. A. Akishin, V. P. Spiridonov, G. A. Sobolev, and V. A. Naumov, Zhur. Fiz. Khim. 31, 1871 (1957).
- JANAF Thermochemical Table: SrBr<sub>2</sub>(g), 6-30-74.
- L. Brewer, G. R. Somayajulu, and E. Brackett, Chem. Rev. 63, 111 (1963).
- B. Rosen, Ed., "Spectroscopic Data Relative to Diatomic Molecules," Pergamon Press, New York, (1970).
- K. S. Krasnov and V. I. Svetsov, Zhv. Vysshikh Uchebn. Zavedenii, Khim. i Khim. Tekhnol. 6, 167 (1963).

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (C <sub>p</sub> <sup>o</sup> - T <sub>r</sub> )/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )/T	Standard State Pressure = P <sup>o</sup> = 0.1 MPa	log K <sub>r</sub>
0	0	INFINITE	INFINITE	-16.542	-271.664
100	56.065	274.673	393.256	-11.858	-271.530
200	60.336	315.227	345.144	-5.983	-273.076
250	61.019	328.771	340.563	-2.948	-273.971
298.15	61.399	339.554	339.554	0	-274.889
300	61.410	339.934	339.555	0.114	-274.926
350	61.653	349.420	340.304	3.191	-276.013
400	61.814	357.664	341.970	6.278	-279.129
450	61.926	364.951	344.126	9.371	-295.470
500	62.007	371.480	346.541	12.470	-337.961
600	62.113	382.796	351.669	18.676	-350.848
700	62.177	392.376	356.817	24.891	-359.025
800	62.220	400.681	361.793	31.111	-363.872
900	62.248	408.011	366.529	37.334	-368.804
1000	62.269	414.571	371.011	43.560	-373.828
1100	62.285	420.507	375.245	49.788	-378.928
1200	62.298	425.927	379.246	56.017	-383.108
1300	62.303	430.914	383.031	62.247	-386.906
1400	62.313	435.531	386.618	68.478	-391.422
1500	62.318	439.830	390.024	74.710	-395.664
1600	62.323	443.853	393.264	80.942	-399.536
1700	62.327	447.631	396.352	87.174	-403.020
1800	62.331	451.194	399.301	93.407	-406.174
1900	62.333	454.564	402.121	99.640	-409.002
2000	62.336	457.761	404.824	105.874	-411.528
2100	62.338	460.803	407.418	112.108	-413.794
2200	62.340	463.703	409.911	118.341	-415.759
2300	62.341	466.474	412.310	124.576	-417.401
2400	62.343	469.127	414.623	130.810	-418.736
2500	62.344	471.672	416.854	137.044	-419.801
2600	62.345	474.117	419.010	143.278	-420.633
2700	62.346	476.470	421.095	149.512	-421.272
2800	62.347	478.757	423.113	155.746	-421.752
2900	62.347	480.925	425.069	161.982	-422.104
3000	62.348	483.039	426.967	168.217	-422.335
3100	62.349	485.083	428.808	174.452	-422.461
3200	62.349	487.063	430.598	180.687	-422.481
3300	62.350	488.981	432.338	186.922	-422.399
3400	62.350	490.843	434.032	193.157	-422.209
3500	62.351	492.650	435.681	199.392	-421.916
3600	62.351	494.407	437.288	205.627	-421.526
3700	62.352	496.115	438.855	211.862	-421.040
3800	62.352	497.778	440.384	218.097	-420.460
3900	62.352	499.397	441.876	224.333	-419.792
4000	62.352	500.976	443.334	230.568	-419.040
4100	62.353	502.516	444.759	236.803	-418.202
4200	62.353	504.018	446.152	243.038	-417.276
4300	62.353	505.488	447.515	249.274	-416.261
4400	62.353	506.919	448.849	255.509	-415.157
4500	62.354	508.320	450.155	261.744	-413.964
4600	62.354	509.691	451.434	267.980	-412.692
4700	62.354	511.032	452.688	274.215	-411.341
4800	62.354	512.344	453.917	280.451	-409.911
4900	62.354	513.630	455.123	286.686	-408.403
5000	62.355	514.890	456.306	292.921	-406.819
5100	62.355	516.125	457.466	299.157	-405.157
5200	62.355	517.335	458.606	305.392	-403.421
5300	62.355	518.523	459.725	311.628	-401.611
5400	62.355	519.689	460.825	317.863	-399.726
5500	62.355	520.833	461.906	324.099	-397.766
5600	62.355	521.956	462.968	330.334	-395.732
5700	62.355	523.060	464.013	336.570	-393.624
5800	62.355	524.145	465.040	342.805	-391.442
5900	62.356	525.210	466.051	349.041	-389.188
6000	62.356	526.259	467.046	355.276	-386.861

PREVIOUS June 1974 (1 atm)

CURRENT: June 1974 (1 bar)

Strontium Iodide (SrI<sub>2</sub>)I<sub>2</sub>Sr<sub>1</sub>(g)

Titanium Iodide (TiI<sub>2</sub>)

CRYSTAL

M<sub>r</sub> = 301.6890

I<sub>2</sub>Ti<sub>1</sub>(cr)

S°(298.15 K) = [122.591 ± 12.6] J·K<sup>-1</sup>·mol<sup>-1</sup>      Δ<sub>f</sub>H°(0 K) = Unknown  
 Δ<sub>f</sub>H°(298.15 K) = -266.10 ± 12.6 kJ·mol<sup>-1</sup>

Enthalpy of Formation

The enthalpy of formation of TiI<sub>2</sub>(cr) is calculated from the enthalpy of reaction for the process 2TiI<sub>2</sub>(cr) = Ti(cr) + TiI<sub>4</sub>(g), and the enthalpy of formation of TiI<sub>4</sub>(cr). Vapor pressure data for this reaction were reported by Herzog and Pidgeon<sup>1</sup> over the temperature range 750 to 902 K. 2nd and 3rd law analyses of these data give values for Δ<sub>f</sub>H°(298.15 K) of 60.5 ± 0.8 and 60.85 kcal·mol<sup>-1</sup>, respectively, the 3rd law drift being 0.4 ± 1.0 cal·K<sup>-1</sup>·mol<sup>-1</sup>. The 3rd law Δ<sub>f</sub>H°(298.15 K) is used to obtain the adopted value of Δ<sub>f</sub>H°(298.15 K).

Heat Capacity and Entropy

The estimated heat capacity is that reported by Kelley.<sup>2</sup> The value of S°(298.15 K) is estimated from that of TiCl<sub>2</sub>(cr) and the difference between ionic entropy contributions of Cl<sup>-</sup> and I<sup>-</sup>.

Sublimation Data

The enthalpy of sublimation of TiI<sub>2</sub>(cr) is taken as the difference in the enthalpies of formation of TiI<sub>2</sub>(cr) and TiI<sub>2</sub>(g) at the sublimation temperature. The sublimation temperature is taken as the point at which Δ<sub>g</sub>G° = 0 for the reaction TiI<sub>2</sub>(cr) = TiI<sub>2</sub>(g).

References

- <sup>1</sup>A. Herzog and L. M. Pidgeon, *Can. J. Chem.*, **34**, 1687 (1956).
- <sup>2</sup>K. K. Kelley, *U. S. Bur. Mines Bull.* **584**, (1961).

T/K	Enthalpy Reference Temperature = T, T = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - [G° - f(T)]/T	H° - H°(T)	Δ <sub>f</sub> H°	
0			0.	-266.102	45.350
100				-266.090	45.063
200				-266.072	44.810
298.15	86.228	122.591	122.591	-255.901	33.417
300	86.241	123.125	122.593	-245.418	25.639
400	86.969	148.034	125.984	-229.934	20.018
500	87.697	167.519	132.412	-214.822	16.030
600	88.425	183.572	139.640	-185.521	10.767
700	89.153	197.258	146.917	-171.258	8.946
800	89.881	209.210	153.973	-157.207	7.465
900	90.609	219.838	160.711	-143.215	6.234
1000	91.337	229.423	167.111	-129.182	5.191
1100	92.065	238.162	173.179	-115.339	4.303
1200	92.793	246.204	178.938	-101.669	3.540
1300	93.521	253.660	184.398	-88.155	2.878
1400	94.249	260.617	189.597	-74.782	2.298
1500	94.977	267.145	194.551	-61.535	1.786
1600	95.705	273.298	199.282	-48.400	1.331
1700	96.433	279.121	203.809	-34.909	0.912
1800	97.161	284.654	208.148		
1900	97.889	289.927	212.315		
2000	98.617	294.966	216.322		

PREVIOUS: June 1964

CURRENT: December 1968

Titanium Iodide (TiI<sub>2</sub>)

I<sub>2</sub>Ti<sub>1</sub>(cr)

## IDEAL GAS

Titanium Iodide (TiI<sub>2</sub>)

$$M_r = 301.6890$$

Titanium Iodide (TiI<sub>2</sub>)

$$S^\circ(298.15 \text{ K}) = [323.673 \pm 16.7] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$\Delta_f H^\circ(0 \text{ K}) = [-17.15 \pm 33.5] \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = [-19.66 \pm 33.5] \text{ kJ} \cdot \text{mol}^{-1}$$

Electronic Levels and Quantum Weights	
$\epsilon$ , cm <sup>-1</sup>	$g$
0	[3]
[7000]	[6]
[17000]	[6]
[22000]	[15]

## Vibrational Frequencies and Degeneracies

$\nu$ , cm <sup>-1</sup>	
[134](1)	
[92](2)	
[290](1)	

Ground State Quantum Weight: [3]

Point Group: [D<sub>∞h</sub>]

Bond Distance: Ti-I = [2.7] Å

Bond Angle: I-Ti-I = [180]°

Rotational Constant: B<sub>0</sub> = [0.009111] cm<sup>-1</sup>

$\sigma = 2$

## Enthalpy of Formation

The enthalpy of formation of TiI<sub>2</sub>(g) is calculated from that of TiI<sub>2</sub>(cr) and the enthalpy of vaporization. Vapor pressure data over the temperature range 750 K to 902 K have been reported by Herzog and Pidgeon<sup>1</sup> and 3rd law analyses of these data give values for  $\Delta_{\text{vap}}H^\circ(298.15 \text{ K})$  of 51.9 and 58.9 kcal·mol<sup>-1</sup>, respectively. The 3rd law drift for these data is 8.3 ± 1.1 cal·K<sup>-1</sup>·mol<sup>-1</sup>, with one point rejected due to failure of a statistical test. The adopted value of  $\Delta_f H^\circ(298.15 \text{ K})$  is calculated from the 3rd law enthalpy of vaporization.

## Heat Capacity and Entropy

The interatomic distances are estimated from those of TiCl<sub>2</sub>(g), TiCl<sub>3</sub>(g), TiBr<sub>2</sub>(g), and TiI<sub>2</sub>(g). The vibrational frequencies are estimated from a valence force field model. The force constant K is estimated as 1.0 millidynes/Å and the constant  $K_0/\lambda^2$  is assumed to be 0.05 millidynes/Å.

The electronic levels are assumed to be the same as TiCl<sub>2</sub>(g). The levels of TiCl<sub>3</sub> are estimated by assuming they correspond to the inverted states of NiCl<sub>2</sub>(g).<sup>2</sup> The linear configuration is adopted, since experimental evidence indicates that other transition metal dihalides are linear.<sup>3,4</sup>

## References

- <sup>1</sup>A. Herzog and L. M. Pidgeon, Can. J. Chem. 34, 1687 (1956).
- <sup>2</sup>C. W. DeKock and D. M. Gruen, J. Chem. Phys. 44, 4387 (1966).
- <sup>3</sup>R. A. Berg and O. Simanoghi, J. Chem. Phys. 32, 1082 (1960).
- <sup>4</sup>J. T. Houghen, G. E. Leroi and T. C. James, J. Chem. Phys. 34, 1670 (1961).
- <sup>5</sup>G. E. Leroi, T. C. James, J. T. Houghen and W. Klemperer, J. Chem. Phys. 36, 2879 (1962).
- <sup>6</sup>A. Buchler, J. L. Stauffer, and W. Klemperer, J. Chem. Phys. 40, 3471 (1964).

I<sub>2</sub>Ti<sub>2</sub>(g)

T/K	C <sub>p</sub> <sup>a</sup>	S <sup>b</sup>	-[C <sub>p</sub> <sup>a</sup> -H <sup>c</sup> (T)]/T	H <sup>c</sup> -H <sup>c</sup> (T)	Δ <sub>f</sub> H <sup>c</sup>	Standard State Pressure = p <sup>d</sup> = 0.1 MPa	log K <sub>r</sub>
	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·mol <sup>-1</sup>	J·mol <sup>-1</sup>	J·mol <sup>-1</sup>	
0	0	0	INFINITE	INFINITE	-17 151	-17 151	INFINITE
100	51.957	261.203	375.991	-11.479	-35.921	-35.921	18.763
200	58.622	279.824	329.167	-17.965	-54.693	-54.693	14.284
250	59.887	313.062	324.667	-18.789	-63.782	-63.782	13.327
298.15	60.570	323.673	323.673	0	-72.369	-72.369	12.679
300	60.591	324.048	323.674	0.112	-72.696	-72.696	12.658
350	61.036	333.424	324.414	3.154	-81.469	-81.469	11.657
400	61.333	341.595	326.062	6.213	-89.495	-89.495	10.811
450	61.542	348.832	328.197	9.283	-96.811	-96.811	10.245
500	61.693	355.324	330.591	12.366	-103.404	-103.404	9.803
600	61.893	366.591	335.680	18.547	-119.409	-119.409	9.277
700	62.016	376.142	340.795	24.742	-134.284	-134.284	8.740
800	62.103	384.429	345.743	30.949	-148.066	-148.066	8.205
900	62.178	391.748	350.456	37.163	-160.777	-160.777	7.677
1000	62.260	398.503	354.919	43.384	-172.453	-172.453	7.151
1100	62.365	404.242	359.137	49.615	-183.098	-183.098	6.636
1200	62.505	409.674	363.125	55.859	-192.726	-192.726	6.122
1300	62.688	414.684	366.901	62.118	-201.343	-201.343	5.610
1400	62.916	419.338	370.482	68.398	-209.000	-209.000	5.100
1500	63.188	423.688	373.886	74.703	-215.729	-215.729	4.593
1600	63.500	427.775	377.127	81.037	-221.543	-221.543	4.090
1700	63.845	431.635	380.221	87.404	-226.453	-226.453	3.591
1800	64.215	435.295	383.180	93.806	-230.466	-230.466	3.097
1900	64.603	438.777	386.015	100.247	-233.607	-233.607	2.608
2000	65.000	442.101	388.737	106.727	-235.900	-235.900	2.124
2100	65.400	445.282	391.355	113.247	-237.353	-237.353	1.645
2200	65.795	448.334	393.876	119.807	-237.976	-237.976	1.171
2300	66.182	451.268	396.308	126.406	-237.763	-237.763	0.702
2400	66.555	454.091	398.657	133.043	-236.717	-236.717	0.239
2500	66.913	456.816	400.929	139.717	-234.855	-234.855	-0.224
2600	67.254	459.447	403.129	146.425	-232.187	-232.187	-0.697
2700	67.579	461.991	405.263	153.167	-228.722	-228.722	-1.171
2800	67.879	464.454	407.333	159.940	-224.466	-224.466	-1.645
2900	68.164	466.841	409.344	166.742	-219.420	-219.420	-2.124
3000	68.431	469.157	411.299	173.572	-213.593	-213.593	-2.608
3100	68.681	471.405	413.202	180.428	-206.997	-206.997	-3.097
3200	68.916	473.589	415.055	187.308	-200.632	-200.632	-3.591
3300	69.137	475.713	416.861	194.211	-193.497	-193.497	-4.090
3400	69.346	477.780	418.623	201.135	-186.592	-186.592	-4.593
3500	69.543	479.793	420.342	208.079	-178.925	-178.925	-5.100
3600	69.730	481.755	422.021	215.043	-170.497	-170.497	-5.610
3700	69.908	483.668	423.661	222.025	-161.311	-161.311	-6.122
3800	70.078	485.534	425.265	229.024	-151.376	-151.376	-6.636
3900	70.242	487.357	426.834	236.040	-140.693	-140.693	-7.151
4000	70.399	489.137	428.369	243.072	-129.263	-129.263	-7.677
4100	70.551	490.877	429.872	250.120	-117.098	-117.098	-8.205
4200	70.697	492.579	431.345	257.182	-104.200	-104.200	-8.740
4300	70.839	494.244	432.789	264.259	-90.564	-90.564	-9.277
4400	70.977	495.875	434.204	271.350	-76.181	-76.181	-9.803
4500	71.110	497.471	435.592	278.455	-61.053	-61.053	-10.328
4600	71.240	499.035	436.955	285.572	-45.185	-45.185	-10.853
4700	71.365	500.569	438.292	292.702	-28.576	-28.576	-11.378
4800	71.486	502.073	439.605	299.845	-11.225	-11.225	-11.903
4900	71.603	503.548	440.899	306.999	6.868	6.868	-12.428
5000	71.716	504.996	442.162	314.165	25.516	25.516	-12.953
5100	71.825	506.417	443.408	321.343	49.763	49.763	-13.478
5200	71.928	507.813	444.634	328.530	79.669	79.669	-14.003
5300	72.028	509.184	445.839	335.728	115.235	115.235	-14.528
5400	72.122	510.531	447.024	342.936	156.463	156.463	-15.053
5500	72.212	511.855	448.191	350.152	203.265	203.265	-15.578
5600	72.296	513.157	449.339	357.378	255.643	255.643	-16.103
5700	72.375	514.437	450.470	364.611	313.597	313.597	-16.628
5800	72.449	515.697	451.584	371.853	377.135	377.135	-17.153
5900	72.517	516.936	452.681	379.101	446.256	446.256	-17.678
6000	72.580	518.155	453.762	386.356	520.921	520.921	-18.203

PREVIOUS: December 1968 (1 atm)

CURRENT: December 1968 (1 bar)

Titanium Iodide (TiI<sub>2</sub>)I<sub>2</sub>Ti<sub>2</sub>(g)

$I_2Zr_1(cr)$

$M_i = 345.0290$  Zirconium Iodide ( $ZrI_2$ )

CRYSTAL

Zirconium Iodide ( $ZrI_2$ )

$S^\circ(298.15\text{ K}) = [150.206] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $T_{\text{fus}} = [700] \text{ K}$

$\Delta_f H^\circ(298.15\text{ K}) = [-259.408] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{liq}} H^\circ = [25.104] \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**

Estimated from a consideration of  $\Delta_f H^\circ(ZrI_4, cr)$  and of the disproportionation data given by Rolsten.<sup>1</sup>

**Heat Capacity and Entropy**

Heat capacity estimated by comparison to the other zirconium halides and titanium halides. Entropy estimated from additive constants.

**Fusion and Vaporization Data**

$\Delta_{\text{liq}} H^\circ$  was estimated.  $T_{\text{fus}}$ ,  $T_{\text{vap}}$  and  $\Delta_{\text{vap}} H^\circ$  from Brewer.<sup>2</sup>

**Reference**

- <sup>1</sup>R. F. Rolsten, "Iodide Metals and Metal Iodides," John Wiley and Sons, Inc., New York, (1961).
- <sup>2</sup>L. Brewer, National Nuclear Energy Series, Div. IV, #9B, paper 7, McGraw-Hill Book Co., Inc., (1950).

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
		S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>r</sub> H <sup>o</sup>	Δ <sub>r</sub> G <sup>o</sup>	
	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	
0			0.			
100						
200						
298.15	94.140	150.206	150.206	-259.408	-257.975	45.196
300	94.349	150.789	150.207	-259.381	-257.966	44.916
400	95.019	178.019	153.915	-274.112	-271.141	33.279
500	95.855	199.313	160.942	-315.389	-288.986	26.009
600	96.699	216.855	168.841	-372.211	-235.980	20.544
700	97.445	231.809	176.794	-385.10	-223.526	16.680
700.000	97.445	231.809	176.794	---	---	---
800	98.157	244.862	184.504	---	---	---
900	99.821	256.520	191.870	---	---	---
1000	99.830	267.022	198.869	---	---	---
1100	100.583	276.571	205.505	---	---	---
1200	101.420	285.359	211.798	---	---	---
1300	102.215	293.509	217.774	---	---	---
1400	103.010	301.113	223.458	---	---	---
1500	103.805	308.247	228.875	---	---	---
				CRYSTAL <--> LIQUID		
				-305.897	-211.524	13.811
				-302.735	-199.917	11.603
				-299.625	-188.661	9.855
				-296.592	-177.712	8.439
				-293.526	-166.815	7.261
				-290.405	-156.079	6.271
				-286.955	-145.609	5.433
				-286.955	-135.387	4.715

PREVIOUS.

CURRENT June 1982

Zirconium Iodide ( $ZrI_2$ )

$I_2Zr_1(cr)$

Zirconium Iodide (ZrI<sub>2</sub>)

$S(K) = [186.168] + K^{-1} \cdot \text{mol}^{-1}$   
 $T_{\text{fus}} = [700] \text{ K}$

Enthalpy of Formation

$\Delta_f H^\circ(\text{ZrI}_2, l, 298.15 \text{ K})$  is calculated from that of the crystal by adding the enthalpy of fusion,  $\Delta_{\text{fus}} H^\circ$ , and the difference in enthalpy,  $H^\circ(700 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and liquid.

Heat Capacity and Entropy

The liquid phase heat capacity is estimated.  $S^\circ(\text{ZrI}_2, l, 298.15 \text{ K})$  is calculated in a manner analogous to that used for the enthalpy of formation.

Fusion and Vaporization Data

$\Delta_{\text{fus}} H^\circ$  was estimated.  $T_{\text{fus}}$ ,  $T_{\text{vap}}$ , and  $\Delta_{\text{vap}} H^\circ$  from Brewer.<sup>1</sup>

Reference

<sup>1</sup>L. Brewer, National Nuclear Energy Series, Div. IV, 19B, paper 7, McGraw Hill Book Co., Inc., (1950).

LIQUID

Zirconium Iodide (ZrI<sub>2</sub>)

I<sub>2</sub>ZrI<sub>3</sub>(l)

Enthalpy Reference Temperature =  $T_r = 298.15 \text{ K}$  Standard State Pressure =  $p^\circ = 0.1 \text{ MPa}$

T/K	$C_p^\circ$	$S^\circ$	$-(G^\circ - H^\circ(T_r))/T$	$H^\circ - H^\circ(T_r)$	$\Delta_f H^\circ$	$\Delta G^\circ$	log K <sub>r</sub>
0							
100							
200							
298.15	94.140	186.168	186.168	0.	-234.239	-243.529	42.665
300	94.349	186.751	186.170	0.174	-234.212	-243.586	42.412
400	95.019	213.982	189.878	9.641	-248.943	-246.357	32.171
500	95.855	235.276	196.904	19.186	-290.220	-241.779	25.258
600	96.609	252.818	204.804	28.808	-287.043	-232.389	20.231
700	97.445	267.672	212.750	38.445	-283.939	-223.526	16.680
700.000	97.445	267.672	212.750	38.445	---	CRYSTAL < -> LIQUID	---
800	106.148	281.251	220.471	48.625	-280.389	-215.128	14.046
900	114.893	294.259	227.951	59.677	-276.075	-207.222	12.077
1000	123.595	306.815	235.213	71.602	-271.008	-199.836	10.433
1100	132.298	319.003	242.279	84.396	-265.200	-192.994	9.165
1200	141.001	330.887	249.170	98.061	-262.369	-186.492	8.118
1300	149.704	342.517	255.905	112.596	-254.559	-180.480	7.252
1400	158.448	353.931	262.500	128.004	-245.949	-175.099	6.533
1500	167.151	365.160	268.971	144.284	-236.560	-170.362	5.933
1600	175.854	376.225	275.329	161.434	-226.413	-166.275	5.428
1700	184.556	387.148	281.586	179.455	-215.529	-162.846	5.004
1800	193.259	397.943	287.751	198.345	-203.925	-160.078	4.645
1900	202.004	408.626	293.832	218.108	-191.613	-157.975	4.343
2000	210.706	419.209	299.837	238.744	-178.604	-156.538	4.088

PREVIOUS.

CURRENT: June 1962

Zirconium Iodide (ZrI<sub>2</sub>)

I<sub>2</sub>ZrI<sub>3</sub>(l)



Zirconium Iodide (ZrI<sub>2</sub>)

IDEAL GAS

M<sub>r</sub> = 345.0290

I<sub>2</sub>Zr<sub>1</sub>(g)

S°(298.15 K) = [344.782] J·K<sup>-1</sup>·mol<sup>-1</sup>      ΔH<sup>0</sup>(0 K) = [-63.262] kJ·mol<sup>-1</sup>  
 ΔH<sup>0</sup>(298.15 K) = [-66.643] kJ·mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies

ν, cm <sup>-1</sup>
[60](1)
[120](1)
[210](1)

Ground State Quantum Weight: [1]  
 Point Group: C<sub>2v</sub>  
 Bond Distance: Zr-I = [2.66] Å  
 Bond Angle: I-Zr-I = 120°  
 Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = 1.072892 × 10<sup>-111</sup> g<sup>3</sup>·cm<sup>6</sup>  
 σ = 2

Enthalpy of Formation

Based upon the estimated value of the ΔH<sup>0</sup> for the crystal and the appropriate crystal and gas functions.

Heat Capacity and Entropy

Molecular constants were all estimated by comparison to similar molecules of zirconium and titanium. The principal moments of inertia are: I<sub>A</sub> = 19.7106 × 10<sup>-39</sup>, I<sub>B</sub> = 223.6596 × 10<sup>-39</sup> and I<sub>C</sub> = 243.3703 × 10<sup>-39</sup> g cm<sup>2</sup>.

T/K	C <sub>p</sub> <sup>0</sup>	S°	[S° - H°(T <sub>0</sub> )]/T	H° - H°(T <sub>0</sub> )	ΔH <sup>0</sup>	log K <sub>r</sub>
Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa				
J·K <sup>-1</sup> ·mol <sup>-1</sup>		J·K <sup>-1</sup> ·mol <sup>-1</sup>		kJ·mol <sup>-1</sup>		
0	0	INFINITE	0	0	-63.262	INFINITE
100	51.686	284.507	0	-15.315	-62.910	83.856
200	56.159	322.118	349.992	-11.026	-64.584	77.216
250	56.834	334.733	345.723	-5.573	-65.500	13.996
298.15	57.238	344.782	347.782	-2.748	-66.643	21.588
300	57.249	345.136	344.783	0	-66.684	21.516
350	57.495	353.981	347.481	0.106	-67.898	19.844
400	57.656	361.670	347.035	2.975	-68.534	18.494
450	57.769	368.468	349.046	5.854	-68.742	17.242
500	57.850	374.558	351.298	8.740	-68.538	15.184
600	57.956	385.116	356.081	17.421	-67.559	13.543
700	58.020	394.055	360.883	24.270	-65.633	11.911
800	58.062	401.806	365.575	29.074	-63.576	10.680
900	58.091	408.646	369.944	34.832	-61.419	9.717
1000	58.112	414.768	374.125	40.642	-59.152	8.940
1100	58.127	420.307	378.076	46.454	-56.774	8.299
1200	58.139	425.366	381.809	52.268	-54.288	7.751
1300	58.148	430.020	385.341	58.082	-51.697	7.279
1400	58.156	434.329	388.688	63.897	-48.999	6.871
1500	58.161	438.342	391.866	69.713	-46.198	6.516
1600	58.166	442.095	394.889	75.530	-43.292	6.202
1700	58.170	445.622	397.771	81.346	-40.281	5.923
1800	58.173	448.947	400.523	87.164	-37.164	5.677
1900	58.176	452.092	403.155	92.981	-33.951	5.446
2000	58.179	455.076	405.677	98.799	-30.642	5.240
2100	58.181	457.915	408.097	104.617	-27.247	5.051
2200	58.182	460.621	410.424	110.435	-23.764	4.859
2300	58.184	463.208	412.663	116.253	-20.193	4.675
2400	58.185	465.684	414.821	122.072	-16.536	4.504
2500	58.187	468.059	416.903	127.890	-12.794	4.345
2600	58.188	470.342	418.915	133.709	-8.964	4.195
2700	58.189	472.538	420.861	139.528	-5.055	4.054
2800	58.190	474.654	422.744	145.347	-1.069	3.921
2900	58.190	476.696	424.570	151.166	2.906	3.796
3000	58.191	478.668	426.340	156.985	6.777	3.677
3100	58.192	480.577	428.059	162.804	10.526	3.564
3200	58.192	482.424	429.729	168.623	14.140	3.457
3300	58.193	484.215	431.353	174.442	17.629	3.355
3400	58.193	485.952	432.934	180.262	21.008	3.257
3500	58.194	487.639	434.473	186.081	24.279	3.165
3600	58.194	489.278	435.973	191.900	27.542	3.076
3700	58.194	490.873	437.435	197.720	30.790	2.990
3800	58.195	492.425	438.862	203.539	34.024	2.909
3900	58.195	493.936	440.255	209.359	37.247	2.831
4000	58.195	495.410	441.615	215.178	40.456	2.756
4100	58.196	496.847	442.945	220.998	43.644	2.683
4200	58.196	498.249	444.245	226.817	46.811	2.614
4300	58.196	499.618	445.517	232.637	49.959	2.547
4400	58.196	500.956	446.762	238.457	53.091	2.483
4500	58.196	502.264	447.981	244.276	56.208	2.420
4600	58.197	503.543	449.175	250.096	59.307	2.360
4700	58.197	504.795	450.345	255.916	62.389	2.303
4800	58.197	506.020	451.492	261.735	65.456	2.250
4900	58.197	507.220	452.617	267.555	68.509	2.200
5000	58.197	508.396	453.721	273.375	71.549	1.770
5100	58.197	509.548	454.804	279.195	74.576	1.605
5200	58.198	510.678	455.868	285.014	77.591	1.445
5300	58.198	511.787	456.913	290.834	80.594	1.292
5400	58.198	512.875	457.939	296.654	83.585	1.144
5500	58.198	513.943	458.947	302.474	86.565	1.001
5600	58.198	514.991	459.939	308.293	89.534	0.863
5700	58.198	516.021	460.914	314.113	92.493	0.729
5800	58.198	517.034	461.873	319.933	95.442	0.600
5900	58.198	518.028	462.816	325.753	98.381	0.473
6000	58.198	519.007	463.744	331.573	101.310	0.354

PREVIOUS: June 1962 (1 atm)

CURRENT: June 1962 (1 bar)

Zirconium Iodide (ZrI<sub>2</sub>)

I<sub>2</sub>Zr<sub>1</sub>(g)



Molybdenum Iodide (MoI<sub>3</sub>)

CRYSTAL

M<sub>r</sub> = 476.6535 Molybdenum Iodide (MoI<sub>3</sub>)

I<sub>3</sub>MoI<sub>1</sub>(cr)

S°(298.15 K) = [195.393 ± 16.7] J·K<sup>-1</sup>·mol<sup>-1</sup>  
 Δ<sub>f</sub>H°(0 K) = Unknown  
 Δ<sub>f</sub>H°(298.15 K) = -124.68 ± 8.4 kJ mol<sup>-1</sup>

Enthalpy of Formation

Barnes *et al.*<sup>1</sup> have measured calorimetrically the enthalpy of formation of MoI<sub>3</sub> by reacting iodine vapor with Mo(CO)<sub>6</sub> at 539 K. The products were found to consist of MoI<sub>2</sub> and Mo by chemical analysis. Assuming a difference in the enthalpies of formation of MoI<sub>3</sub> and MoI<sub>2</sub> of 1.5 kcal·mol<sup>-1</sup>, Barnes *et al.*<sup>1</sup> determined that the Δ<sub>f</sub>H°(MoI<sub>3</sub>, cr, 298.15 K) = 26.2 ± 2.0 kcal·mol<sup>-1</sup>. Brewer<sup>2</sup> has estimated that the difference Δ<sub>f</sub>H°(MoI<sub>3</sub>)Δ<sub>f</sub>H°(MoI<sub>2</sub>) may be as large as -5 kcal mol<sup>-1</sup> and reanalyzed the heat of iodination data with the result Δ<sub>f</sub>H°(MoI<sub>3</sub>, cr, 298.15 K)/R = -15000 ± 1000 K which is adopted. We adopt the estimate of Brewer.<sup>2</sup> The assigned uncertainty (±2.0 kcal·mol<sup>-1</sup>) is determined from the product 1000 × R which has been rounded to the nearest kcal mol<sup>-1</sup>.

Heat Capacity and Entropy

The values of S°(298.15 K) and C<sub>p</sub>° over the temperature range 298–1000 K are estimates reported by Brewer.<sup>2</sup> We treat the estimated entropy value given as S°(298.15 K)/R in a manner similar to that for the enthalpy of formation.

Phase Data

Drobot *et al.*<sup>3</sup> have studied the thermal decomposition of MoI<sub>3</sub> in evacuated sealed ampoules at various temperatures. X-ray diffraction and chemical analyses of the condensed decomposition products showed the existence of a homogeneity range in which the atomic ratio of I/Mo varied from 3.00 to 2.5. The crystal structure of MoI<sub>3</sub> is of P16<sup>2</sup> in the Pearson classification system.

Decomposition Data

T<sub>dec</sub> of 629.5 K is calculated as the decomposition temperature at which the fugacity of iodine is 1 atm for the dissociation reaction MoI<sub>3</sub>(cr) = MoI<sub>2</sub>(cr) + 0.5 I<sub>2</sub>(g). Saturated vapor pressure measurements by Drobot *et al.*<sup>3</sup> indicate that MoI<sub>3</sub>(cr) decomposes to a non stoichiometric triiodide phase beginning at a temperature near 363.2 K.

References

- <sup>1</sup>D. S. Barnes, G. Pilcher, D. A. Pittam, H. A. Skinner, D. Todd, and Y. Virman, *J. Less Common Met.* **36**, 177 (1974).
- <sup>2</sup>L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal communication, September 29, 1978, preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria.
- <sup>3</sup>D. V. Drobot, L. G. Mikhailova, K. A. Bol'shakov, and V. L. Sbitnev, *Russ. J. Inorg. Chem.* **23**, (5), 643 (1978).

T/K	Enthalpy Reference Temperature = T, = 298.15 K			Standard State Pressure = p° = 0.1 MPa		
	C <sub>p</sub> <sup>o</sup>	S° - [G° - H°(T)]/T	H° - H°(T)	Δ <sub>f</sub> H°	Δ <sub>f</sub> G°	log K <sub>r</sub>
0			0.			
100						
200						
298.15	108.889	195.393	195.393	-124.683	-122.469	21.456
300	108.918	196.066	195.395	-124.677	-122.456	21.321
400	110.583	227.628	199.687	-148.615	-170.905	15.789
500	112.244	252.483	207.847	-212.317	-107.872	11.269
600	113.909	273.094	217.052	-209.257	-87.269	7.597
700	115.570	290.778	226.350	-206.107	-67.185	5.013
800	117.231	306.319	235.394	-202.857	-47.559	3.105
900	118.897	320.223	244.061	-199.502	-28.347	1.645
1000	120.558	332.836	252.317	-196.045	-9.515	0.497

PREVIOUS:

CURRENT: September 1978

Molybdenum Iodide (MoI<sub>3</sub>)

I<sub>3</sub>MoI<sub>1</sub>(cr)

Molybdenum Iodide (MoI<sub>3</sub>)

IDEAL GAS

M<sub>r</sub> = 476.6535

I<sub>3</sub>Mo<sub>1</sub>(g)

S°(298.15 K) = {403.532 ± 8.4} J·K<sup>-1</sup>·mol<sup>-1</sup>

ΔH<sup>o</sup>(0 K) = [186.15 ± 41.8] kJ·mol<sup>-1</sup>  
 ΔH<sup>o</sup>(298.15 K) = [182.84 ± 41.8] kJ·mol<sup>-1</sup>

Electronic Levels and Quantum Weights	
ε <sub>e</sub> , cm <sup>-1</sup>	g <sub>e</sub>
[0]	2
[3505.4]	2
[10861.0]	4
[11062.0]	4

Vibrational Frequencies and Degeneracies	
ν <sub>i</sub> , cm <sup>-1</sup>	
[110](1)	
[75](1)	
[200](2)	
[60](2)	

Point Group: [D<sub>3h</sub>]  
 Bond Distance: Mo-I = [2.66] Å  
 Bond Angle: I-Mo-I = [120]°  
 Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [2.237654 × 10<sup>-110</sup>] g<sup>3</sup>·cm<sup>6</sup>  
 σ = [6]

Enthalpy of Formation

The adopted value of Δ<sub>f</sub>H<sup>o</sup> at 298.15 K is that estimated by Brewer.<sup>1</sup> The estimated value is consistent with the low volatility of solid molybdenum in iodine vapor reported by Schafer *et al.*<sup>2</sup> The estimated value given by Brewer is Δ<sub>f</sub>H<sup>o</sup>(298.15 K)/R = 22000 ± 5000 K. The assigned uncertainty (± 10 kcal mol<sup>-1</sup>) is determined from the product 5000 × R which has been rounded to the nearest kcal·mol<sup>-1</sup>. The value of Δ<sub>f</sub>H<sup>o</sup>(0 K) combined with JANAF data for Mo(g) and I(g) gives Δ<sub>f</sub>H<sup>o</sup>(0 K) = 189 ± 11 kcal·mol<sup>-1</sup> and an average Mo-I bond energy of Δ<sub>b</sub>H<sup>o</sup>(0 K)/3 = 63 ± 4 kcal·mol<sup>-1</sup>.

Heat Capacity and Entropy

The bond length and vibrational frequencies are values estimated by Brewer.<sup>1</sup> A planar structure has been predicted for MoI<sub>3</sub> by Drake and Rosenblatt.<sup>4</sup> The electronic contribution is taken to be the same as that for TaO, as estimated by Brewer.<sup>1</sup> The levels are taken from the latest JANAF table<sup>3</sup> however, we only include four levels. The principal moments of inertia are: I<sub>A</sub> = I<sub>B</sub> = 223.6596 × 10<sup>-39</sup>, and I<sub>C</sub> = 447.3193 × 10<sup>-39</sup> g·cm<sup>2</sup>.

References

- L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley; personal communication, September 29, 1978, preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria.
- H. Schafer, T. Grofe, and M. Trenkel, *J. Solid State Chem.* **8**, 14 (1973).
- JANAF Thermochemical Tables: Mo(g), 3-31-78; I(g), 3-30-74; TaO(g), 12-31-73.
- M. C. Drake and G. M. Rosenblatt, Paper 388, The Electrochemical Society, Atlanta, Georgia, (October 1977).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>i</sub>
	C <sub>p</sub> <sup>o</sup>	S° - [C <sub>p</sub> <sup>o</sup> (T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	Δ <sub>f</sub> G°	
	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·K <sup>-1</sup> ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	
0	0	INFINITE	0	186.152	INFINITE
100	71.920	318.351	-21.071	186.546	-85.958
200	79.674	371.309	-7.927	184.989	-37.377
250	80.859	389.229	-3.910	183.946	-27.758
298.15	81.513	403.532	0	182.841	-21.549
300	81.532	404.036	0.151	182.796	-21.351
350	81.949	416.638	4.239	181.452	-17.700
400	82.227	427.600	8.343	156.076	-13.554
450	82.427	437.297	12.460	152.878	-11.312
500	82.585	445.990	16.585	149.474	-9.115
600	82.861	461.072	24.858	140.701	-6.593
700	83.159	473.867	33.159	132.316	-4.783
800	83.514	484.954	41.492	124.236	-3.426
900	83.914	494.853	49.863	116.304	-2.405
1000	84.342	503.716	58.275	108.457	-1.645
1100	84.772	511.775	66.731	100.777	-1.112
1200	85.185	519.169	75.229	93.338	-0.749
1300	85.582	526.002	83.767	86.068	-0.485
1400	85.966	532.356	92.340	78.972	-0.283
1500	86.214	538.294	100.947	72.048	-0.121
1600	86.492	543.867	109.582	65.272	0.000
1700	86.745	549.118	118.244	58.648	0.100
1800	86.980	554.083	126.931	52.168	0.180
1900	87.205	558.792	135.640	45.836	0.240
2000	87.425	563.270	144.371	39.548	0.280
2100	87.644	567.541	153.125	33.300	0.300
2200	87.865	571.624	161.900	27.092	0.310
2300	88.090	575.534	170.698	20.924	0.310
2400	88.318	579.288	179.519	14.796	0.300
2500	88.550	582.898	188.362	8.708	0.280
2600	88.784	586.376	197.229	2.660	0.250
2700	89.018	589.731	206.119	-3.340	0.210
2800	89.255	592.972	215.032	-9.460	0.160
2900	89.479	596.108	223.969	-15.610	0.100
3000	89.702	599.146	232.928	-21.780	0.030
3100	89.917	602.090	241.909	-27.970	-0.040
3200	90.122	604.948	250.911	-34.180	-0.110
3300	90.316	607.725	259.933	-40.410	-0.180
3400	90.498	610.424	268.973	-46.660	-0.250
3500	90.666	613.049	278.032	-52.930	-0.320
3600	90.819	615.606	287.106	-59.220	-0.390
3700	90.957	618.096	296.195	-65.530	-0.460
3800	91.081	620.523	305.297	-71.860	-0.530
3900	91.188	622.890	314.411	-78.210	-0.600
4000	91.280	625.200	323.534	-84.580	-0.670
4100	91.357	627.455	332.666	-90.970	-0.740
4200	91.418	629.658	341.805	-97.380	-0.810
4300	91.466	631.809	350.949	-103.810	-0.880
4400	91.499	633.912	360.098	-110.260	-0.950
4500	91.519	635.969	369.249	-116.730	-1.020
4600	91.527	637.980	378.401	-123.220	-1.090
4700	91.522	639.949	387.554	-129.730	-1.160
4800	91.507	641.876	396.705	-136.260	-1.230
4900	91.481	643.762	405.855	-142.810	-1.300
5000	91.446	645.610	415.001	-149.380	-1.370
5100	91.402	647.420	424.144	-155.970	-1.440
5200	91.349	649.195	433.281	-162.580	-1.510
5300	91.290	650.934	441.413	-169.210	-1.580
5400	91.223	652.640	449.539	-175.860	-1.650
5500	91.151	654.313	457.657	-182.530	-1.720
5600	91.073	655.955	465.769	-189.220	-1.790
5700	90.991	657.566	473.872	-195.930	-1.860
5800	90.904	659.148	481.967	-202.660	-1.930
5900	90.813	660.701	489.053	-209.410	-2.000
6000	90.720	662.227	496.129	-216.180	-2.070

PREVIOUS: September 1978 (1 atm)

CURRENT: September 1978 (1 bar)

Molybdenum Iodide (MoI<sub>3</sub>)

I<sub>3</sub>Mo<sub>1</sub>(g)

Triiodosilyl (SiI<sub>3</sub>)

IDEAL GAS

M<sub>r</sub> = 408.7990 Triiodosilyl (SiI<sub>3</sub>)

I<sub>3</sub>Si(g)

$\Delta_f H^\circ(0\text{ K}) = [378.305 \pm 8.4] \text{ J}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = [35.31 \pm 62.8] \text{ kJ}\cdot\text{mol}^{-1}$

Standard State Pressure =  $p^\circ = 0.1\text{ MPa}$

Vibrational Frequencies and Degeneracies  
 $\nu, \text{ cm}^{-1}$   
 [286](1)  
 [122](1)  
 [399](2)  
 [80](2)

Ground State Quantum Weight: [2]  
 Point Group: [C<sub>3v</sub>]  
 Bond Distance: Si-I = [2.435] Å  
 Bond Angle: I-Si-I = [112]<sup>o</sup>  
 Product of the Moments of Inertia:  $I_A I_B I_C = [1.038908 \times 10^{-110}] \text{ g}^3\cdot\text{cm}^6$   
 $\sigma = [3]$

Enthalpy of Formation

The enthalpy of formation of SiI<sub>3</sub>(g) is based on an assumed average bond energy of  $58 \pm 5 \text{ kcal}\cdot\text{mol}^{-1}$ . This average bond energy is that of SiI (g), i.e.  $\Delta_f H^\circ(\text{SiI}_4, \text{ g}, 0\text{ K})/4$ . The rationale for this assumption is based on the same relationship existing for the silicon chloride and fluoride species.<sup>1</sup>

Heat Capacity and Entropy

The molecular structure is assumed to be identical to the SiI<sub>3</sub> group in SiH<sub>3</sub>.<sup>1</sup> From this structure we estimate the following principal moments of inertia:  $I_A = I_B = 173.9077 \times 10^{-39}$ , and  $I_C = 343.5099 \times 10^{-39} \text{ g}\cdot\text{cm}^2$ . The vibrational frequencies are assumed to be those of the SiI<sub>3</sub> group in SiH<sub>3</sub>(g).

Reference

<sup>1</sup>JANAF Thermochemical Tables: SiI<sub>3</sub>(g), SiCl<sub>3</sub>(g) and SiF<sub>3</sub>(g), 12-31-77; SiH<sub>3</sub>(g), 12-31-76.

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )]/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>f</sub> H <sup>o</sup>	
0	0	0	INFINITE	INFINITE	
100	58.786	303.097	-18.578	39.751	INFINITE
200	71.873	348.463	-13.974	30.514	-0.987
250	75.152	364.881	-7.353	37.557	-0.345
298.15	77.191	378.305	-5.071	36.448	-0.279
300	77.254	378.783	0	35.514	3.491
350	78.652	390.803	0.143	35.268	3.529
400	79.619	401.373	0.403	33.916	4.391
450	80.310	410.793	8.001	8.548	4.904
500	80.820	419.282	12.000	5.373	5.006
600	81.503	434.083	16.029	-57.997	4.455
700	81.926	446.681	397.836	-57.885	3.446
800	82.206	457.640	400.508	-57.811	2.727
900	82.399	467.334	406.979	-57.781	2.188
1000	82.539	476.023	413.157	-57.798	1.788
1100	82.643	483.895	419.017	-57.864	1.433
1200	82.722	491.090	424.563	-57.984	1.158
1300	82.784	497.714	429.811	-58.163	0.928
1400	82.833	503.850	434.783	-58.412	0.733
1500	82.873	509.567	439.500	-58.744	0.565
1600	82.906	514.916	443.983	-59.174	0.418
1700	82.933	519.943	448.251	-59.717	0.289
1800	82.955	524.684	452.371	-110.563	0.160
1900	82.975	529.170	456.211	-111.100	-0.030
2000	82.991	533.426	460.503	-111.488	-0.200
2100	83.005	537.476	465.200	-111.600	-0.354
2200	83.018	541.338	470.325	-113.482	-0.623
2300	83.028	545.028	475.398	-114.456	-0.955
2400	83.038	548.562	480.456	-115.511	-1.472
2500	83.046	551.952	485.499	-116.632	-2.142
2600	83.053	555.209	490.529	-117.804	-2.954
2700	83.060	558.344	495.546	-119.008	-3.949
2800	83.066	561.365	500.544	-120.227	-5.138
2900	83.071	564.280	505.526	-121.444	-6.582
3000	83.076	567.096	510.496	-122.644	-8.279
3100	83.080	569.820	515.441	-123.811	-10.374
3200	83.084	572.458	520.366	-124.933	-12.844
3300	83.088	575.014	525.276	-126.000	-15.710
3400	83.091	577.495	530.166	-127.000	-18.937
3500	83.094	579.904	535.032	-127.928	-22.568
3600	83.097	582.244	540.000	-128.777	-26.639
3700	83.099	584.521	545.083	-129.641	-31.189
3800	83.102	586.737	550.276	-130.504	-36.266
3900	83.104	588.896	555.570	-131.361	-41.921
4000	83.106	591.000	560.961	-132.212	-48.167
4100	83.108	593.052	566.441	-133.056	-55.032
4200	83.109	595.055	572.016	-133.891	-62.529
4300	83.111	597.010	577.684	-134.717	-70.659
4400	83.112	598.921	583.441	-135.533	-79.418
4500	83.114	600.789	589.289	-136.339	-88.799
4600	83.115	602.616	595.226	-137.136	-98.883
4700	83.116	604.403	601.256	-137.923	-109.668
4800	83.117	606.153	607.374	-138.699	-121.144
4900	83.119	607.867	613.586	-139.464	-133.399
5000	83.120	609.546	619.889	-140.217	-146.418
5100	83.121	611.192	626.289	-140.958	-160.183
5200	83.121	612.806	632.789	-141.687	-174.683
5300	83.122	614.390	639.394	-142.404	-189.899
5400	83.123	615.943	646.119	-143.109	-205.806
5500	83.124	617.469	652.969	-143.801	-222.389
5600	83.125	618.966	660.000	-144.481	-239.614
5700	83.125	620.438	667.226	-145.148	-257.459
5800	83.126	621.883	674.654	-145.801	-275.899
5900	83.126	623.304	682.289	-146.441	-294.906
6000	83.127	624.701	690.000	-147.067	-314.459

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

Triiodosilyl (SiI<sub>3</sub>)

I<sub>3</sub>Si(g)

CRYSTAL

Titanium Iodide (TiI<sub>3</sub>)

M<sub>r</sub> = 428.5935

Titanium Iodide (TiI<sub>3</sub>)

I<sub>3</sub>Ti<sub>3</sub>(cr)

S<sup>o</sup>(298.15 K) [192.464 ± 8.4] J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>sub</sub> = [1000] K  
 $\Delta_f H^\circ(0 \text{ K}) = \text{Unknown}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = [-322.17 \pm 20.9] \text{ kJ}\cdot\text{mol}^{-1}$

Enthalpy of Formation

The enthalpy of formation of TiI<sub>3</sub>(cr) is calculated from the free energy of formation at 623 K combined with the increment  $\Delta_f G^\circ(623 \text{ K})$  ( $\Delta_f G^\circ(298.15 \text{ K})$  and the entropies, S<sup>o</sup>(298.15 K), of TiI<sub>4</sub>(cr), TiI<sub>3</sub>(cr) and TiI<sub>2</sub>(g). The free energy of formation,  $\Delta_f G^\circ(623 \text{ K})$ , is estimated such that  $\Delta_f G^\circ(623 \text{ K}) = 0$  for the process 2TiI<sub>3</sub>(cr) = TiI<sub>2</sub>(cr) + TiI<sub>4</sub>(g). This assumption is based on the observations of Herczog and Pidgeon<sup>1</sup> and Fast<sup>2</sup>.

Heat Capacity and Entropy

The heat capacities of TiI<sub>3</sub>(cr) and the value of S<sup>o</sup>(298.15 K) estimated by Kelley<sup>3</sup> have been adopted.

Sublimation Data

The enthalpy of sublimation of TiI<sub>3</sub>(cr) is taken as the difference in the enthalpies of formation of TiI<sub>3</sub>(cr) and TiI<sub>3</sub>(g) at the sublimation temperature. The sublimation temperature is estimated as the point at which  $\Delta_f G^\circ = 0$  for the process TiI<sub>3</sub>(cr) = TiI<sub>3</sub>(g).

References

- <sup>1</sup>A. Herczog and L. M. Pidgeon, *Can. J. Chem.* **34**, 1687 (1956).
- <sup>2</sup>J. P. Fast, *Rec. Trav. Chim.* **58**, 174 (1939).
- <sup>3</sup>K. K. Kelley, *U. S. Bur. Mines Bull.* **584**, 232 pp. 1960; *U. S. Bur. Mines Bull.* **592**, 149 pp. (1961).

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup>	-[G <sup>o</sup> -H <sup>o</sup> (T)]/T	H <sup>o</sup> -H <sup>o</sup> (T)	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K <sub>f</sub>
Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K							
Standard State Pressure = p <sup>o</sup> = 0.1 MPa							
KJ·mol <sup>-1</sup>							
0							
100							
200							
298.15	116.771	192.464	192.464	0	-322.168	-318.439	55.789
300	116.784	193.186	192.466	0.216	-322.150	-318.416	55.441
400	117.512	226.883	197.056	11.931	-345.506	-316.453	41.324
500	118.240	253.183	205.746	23.718	-408.753	-303.138	31.669
600	118.968	274.805	215.507	35.579	-405.350	-282.335	24.579
700	119.696	293.199	225.324	47.512	-401.956	-262.101	19.538
800	120.424	309.229	234.832	59.518	-398.543	-242.354	15.824
900	121.152	323.455	243.903	71.597	-395.141	-223.035	12.945
1000	121.880	336.257	252.509	83.748	-391.813	-204.092	10.681
1100	122.608	347.908	260.660	95.973	-388.627	-185.476	8.808
1200	123.336	358.607	268.583	108.270	-385.573	-167.022	7.270
1300	124.064	368.508	275.708	120.640	-382.648	-148.623	5.972
1400	124.792	377.729	282.670	133.083	-382.414	-130.499	4.869
1500	125.520	386.564	289.298	145.598	-378.940	-112.627	3.922

PREVIOUS: June 1964

CURRENT: December 1968

Titanium Iodide (TiI<sub>3</sub>)

I<sub>3</sub>Ti<sub>3</sub>(cr)

Titanium Iodide (TiI<sub>3</sub>)

IDEAL GAS

M<sub>r</sub> = 428.5935 Titanium Iodide (TiI<sub>3</sub>)

I<sub>3</sub>TiI<sub>3</sub>(g)

$\Delta_f H^\circ(0 \text{ K}) = [-144.51 \pm 33.5] \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = [-150.21 \pm 33.5] \text{ kJ}\cdot\text{mol}^{-1}$

Electronic Levels and Quantum Weights	$\epsilon_i, \text{cm}^{-1}$	$g_i$
0	[2]	4000 [2]
600	[2]	10000 [2]
1500	[2]	

Vibrational Frequencies and Degeneracies	$\nu_i, \text{cm}^{-1}$	$\nu_i$
	[341](1)	(383)(2)
	[123](1)	[74](2)

Ground State Quantum Weight: [2]  
 Point Group: [C<sub>3v</sub>]  
 Bond Distance: Ti-I = [2.7] Å  
 Bond Angle: I-Ti-I = [100]°  
 Product of the Moments of Inertia:  $I_A I_B I_C = 1.322449 \times 10^{-107} \text{ g}^3 \cdot \text{cm}^6$

Enthalpy of Formation

The enthalpy of formation,  $\Delta_f H^\circ(\text{TiI}_3, g, 298.15 \text{ K})$ , is estimated from the average Ti-I bond energy. The bond energy is estimated from the corresponding quantities for TiBr<sub>3</sub>(g), TiBr<sub>3</sub>(g) and TiI<sub>4</sub>(g).

Heat Capacity and Entropy

The interatomic distance is estimated from those of TiI<sub>4</sub>, TiCl<sub>4</sub> and TiCl<sub>3</sub>. The pyramidal bond angle is estimated by assuming that TiI<sub>3</sub>(g) is similar to the group V trihalides. The principal moments of inertia are:  $I_A = I_B = 191.5028 \times 10^{-39}$  and  $I_C = 360.6023 \times 10^{-39} \text{ g}\cdot\text{cm}^2$ . The vibrational frequencies are estimated from valence force field predictions and comparisons with group V trihalides. The electronic levels are estimated from the levels of Ti<sup>3+</sup> reported by Moore.<sup>1</sup>

Reference

<sup>1</sup>C. E. Moore, U. S. Nat. Bur. Stand. Circ. 467, (1949).

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	Δ <sub>f</sub> H <sup>o</sup>	Δ <sub>f</sub> G <sup>o</sup>	log K <sub>r</sub>
0	0.	INFINITE	-18.933	-144.511	-144.511	INFINITE
100	38.519	305.563	448.602	-143.004	-145.018	86.500
200	73.632	351.232	389.367	-145.304	-147.657	86.500
250	78.018	368.168	383.480	-147.657	-148.963	86.500
298.15	80.800	382.164	382.164	0.	-203.035	35.571
300	80.886	382.664	382.166	0.150	-203.363	35.409
350	82.769	395.284	383.158	4.244	-212.107	31.654
400	84.024	406.424	385.384	8.416	-219.822	28.706
450	84.870	416.373	388.284	12.640	-224.976	26.114
500	85.440	425.346	391.549	16.899	-224.077	23.409
600	86.063	440.987	398.523	25.478	-220.183	19.169
700	86.303	454.275	405.563	34.099	-216.305	16.141
800	86.363	465.804	412.388	42.733	-213.407	13.871
900	86.344	475.976	418.900	51.369	-210.570	12.105
1000	86.297	485.071	425.070	60.001	-208.690	10.692
1100	86.242	493.293	430.904	68.628	-207.782	9.534
1200	86.187	500.795	436.420	77.249	-206.832	8.562
1300	86.133	507.691	441.641	85.865	-205.870	7.730
1400	86.083	514.073	446.590	94.476	-204.958	7.015
1500	86.034	520.010	451.289	103.082	-204.094	6.395
1600	85.988	525.561	455.759	111.683	-203.282	5.852
1700	85.943	530.773	460.020	120.279	-202.513	5.371
1800	85.900	535.684	464.088	128.871	-201.788	4.941
1900	85.860	540.327	467.980	137.459	-201.109	4.556
2000	85.822	544.730	471.708	146.044	-200.469	4.194
2100	85.787	548.917	475.286	154.624	-199.866	3.858
2200	85.754	552.907	478.724	163.201	-199.298	3.548
2300	85.723	556.718	482.033	171.775	-198.763	3.263
2400	85.695	560.366	485.221	180.346	-198.263	2.999
2500	85.669	563.863	488.298	188.914	-197.788	2.754
2600	85.644	567.223	491.269	197.479	-197.342	2.525
2700	85.622	570.455	494.142	206.043	-196.924	2.310
2800	85.600	573.568	496.924	214.604	-196.535	2.109
2900	85.580	576.571	499.619	223.163	-196.166	1.920
3000	85.561	579.472	502.232	231.720	-195.820	1.742
3100	85.543	582.278	504.770	240.275	-195.494	1.574
3200	85.525	584.993	507.234	248.829	-195.186	1.415
3300	85.507	587.625	509.631	257.380	-194.893	1.264
3400	85.490	590.177	511.962	265.930	-194.614	1.120
3500	85.473	592.655	514.233	274.478	-194.349	0.984
3600	85.456	595.063	516.445	283.025	-194.096	0.854
3700	85.439	597.404	518.601	291.569	-193.854	0.729
3800	85.422	599.682	520.705	300.112	-193.623	0.609
3900	85.404	601.901	522.759	308.654	-193.399	0.494
4000	85.386	604.063	524.764	317.193	-193.182	0.384
4100	85.369	606.171	526.724	325.731	-192.971	0.279
4200	85.350	608.228	528.641	334.267	-192.766	0.179
4300	85.332	610.236	530.515	342.801	-192.566	0.084
4400	85.313	612.198	532.349	351.333	-192.371	0.016
4500	85.294	614.115	534.145	359.864	-192.181	-0.041
4600	85.275	615.989	535.904	368.392	-191.996	-0.096
4700	85.255	617.823	537.627	376.919	-191.816	-0.151
4800	85.235	619.617	539.317	385.443	-191.641	-0.206
4900	85.215	621.375	540.974	393.966	-191.471	-0.261
5000	85.195	623.096	542.599	402.486	-191.306	-0.316
5100	85.174	624.783	544.194	411.005	-191.146	-0.371
5200	85.154	626.437	545.760	419.521	-190.991	-0.426
5300	85.133	628.059	547.297	428.035	-190.840	-0.481
5400	85.112	629.650	548.808	436.548	-190.693	-0.536
5500	85.091	631.211	550.292	445.058	-190.550	-0.591
5600	85.070	632.744	551.750	453.566	-190.411	-0.646
5700	85.049	634.250	553.185	462.072	-190.276	-0.701
5800	85.028	635.729	554.595	470.576	-190.145	-0.756
5900	85.007	637.182	555.983	479.077	-190.018	-0.811
6000	84.986	638.611	557.348	487.577	-189.895	-0.866

PREVIOUS: December 1968 (1 atm)

CURRENT: December 1968 (1 bar)

Titanium Iodide (TiI<sub>3</sub>)

I<sub>3</sub>TiI<sub>3</sub>(g)

Zirconium Iodide (ZrI<sub>3</sub>)

## CRYSTAL

M<sub>r</sub> = 471.9335Zirconium Iodide (ZrI<sub>3</sub>)I<sub>3</sub>Zr<sub>1</sub>(cr)

$$S^{\circ}(298.15 \text{ K}) = [204.585] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{sub}} = [970] \text{ K}$$

$$\Delta H_f^{\circ}(0 \text{ K}) = [-396.545] \text{ kJ} \cdot \text{mol}^{-1}$$

$$\Delta H_f^{\circ}(298.15 \text{ K}) = [-397.480] \text{ kJ} \cdot \text{mol}^{-1}$$

## Enthalpy of Formation

Larsen and Leddy<sup>1</sup> studied the reaction  $\text{Zr}(\text{cr}) + 3 \text{ZrI}_2(\text{g}) = 4 \text{ZrI}_3(\text{cr})$  in the temperature range 473 to 973 K and pressure range 5 to 15 atm. They present a plot of the fractional reaction, at a number of temperatures, as a function of reaction time, however, they express doubt concerning the attainment of thermodynamic equilibrium.

The Gibbs energy function change for this reaction was calculated at 100 K from 500 to 1100 K. At each temperature the equilibrium constant was assumed to be 1, and  $\Delta H_f^{\circ}(298.15 \text{ K})$  accordingly calculated. These values and the enthalpy of formation of  $\text{ZrI}_4(\text{g})$  [see  $\text{ZrI}_4$  table] were used to compute a series of values for the enthalpy of formation of  $\text{ZrI}_3(\text{cr})$  at 298.15 K. The following table gives representative values at four temperatures.

T/K	K <sub>p</sub>	$\Delta H_f^{\circ}(298.15 \text{ K}), \text{ kcal} \cdot \text{mol}^{-1}$	$\Delta H_f^{\circ}(298.15 \text{ K}), \text{ kcal} \cdot \text{mol}^{-1}$
500	1	-66.0	-80.2
700	1	-90.3	-86.2
900	1	-113.5	-92.1
1100	1	-135.9	-97.7

If one assumes an initial pressure of from 5 to 10 atm. for  $\text{ZrI}_4$  and stoichiometric amounts of reactants, then, on the basis of zirconium, the reaction must proceed to the extent of 80 to 90% for the pressure of  $\text{ZrI}_4$  to attain a value of 1 atm. and hence an equilibrium constant of 1. The data of Larsen and Leddy indicate that the reaction proceeds to the extent of 88% at 973 K. From this it was assumed that at around 1000 K the equilibrium constant attains a value of 1 giving  $-95 \text{ kcal} \cdot \text{mol}^{-1}$  for the enthalpy of formation of  $\text{ZrI}_3$  at 298.15 K.

Their data were subjected to a 2nd law calculation but the results are of doubtful value in view of the uncertainty in the attainment of thermodynamic equilibrium at the lower temperature. The limits of error assigned to the enthalpy of formation are  $\pm 15 \text{ kcal} \cdot \text{mol}^{-1}$  corresponding to a temperature spread of  $\pm 500$  in the above table.

## Heat Capacity and Entropy

The heat capacity was estimated in the same manner as for  $\text{ZrBr}_4(\text{cr})$  [refer to the  $\text{ZrBr}_4(\text{cr})$  table]. The value  $\theta_D = 60 \text{ K}$  and  $\theta_E = 115 \text{ K}$  were taken to be the same as those estimated for  $\text{ZrI}_4(\text{cr})$ . The internal contribution was obtained from the estimated  $\text{ZrI}_3$  vibrational frequencies and the anharmonicity factor "a" was taken to be  $2.5 \times 10^{-3}$ . The specific heat above 300 K was obtained by graphical extrapolation.

For the above estimation, it was assumed that the crystalline lattice is made up of  $\text{ZrI}_3$  molecules. However, Holze<sup>2</sup> came to the conclusion that crystalline  $\text{ZrI}_3$  is composed of a chain lattice of  $(\text{Zr}_2\text{I}_6)_n$  units. The results of an analysis for a crystalline lattice composed of  $\text{Zr}_2\text{I}_6$  units would probably not differ significantly from that for a crystalline lattice composed of  $\text{ZrI}_3$  units since both are approaching the classical harmonic heat capacity of 12R calories per formula weight of  $\text{ZrI}_3$  at relatively low temperatures.

Until more quantitative information becomes available, it is felt that the above analysis gives a fair approximation to the heat capacity of  $\text{ZrI}_3$ .

## Decomposition Data

A's described in the "Enthalpy of Formation" section, the temperature of decomposition was assumed to be  $1000 \pm 500 \text{ K}$ .

## Liquid Data

It is assumed that the liquid phase is thermodynamically unstable under ordinary conditions.

## Sublimation Data

The enthalpy of sublimation at 298.15 K was obtained from the difference in the enthalpies of formation of the gas and solid at 298.15 K. The sublimation point was obtained from the free energy crossover between gas and solid.

## References

- <sup>1</sup>E. M. Larsen and J. J. Leddy, *J. Amer. Chem. Soc.* **78**, 5983 (1956).
- <sup>2</sup>E. Holze, see R. F. Rolsten, "Iodide Metals and Metal Iodides," John Wiley & Sons, Inc., New York, 46, (1961).

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup>	$-(G^{\circ} - H^{\circ}(T))/T$	$H^{\circ} - H^{\circ}(T)$	$\Delta H_f^{\circ}$	$\Delta G_f^{\circ}$	log K <sub>f</sub>
0	0	0	INFINITE	-24.359	-396.545	-396.545	INFINITE
100	83.366	100.663	292.625	-19.196	-396.843	-396.555	207.035
200	98.328	164.189	213.936	-9.950	-397.188	-395.728	103.354
298.15	103.818	204.585	204.585	0	-397.480	-394.947	69.193
300	103.897	205.227	204.587	0.192	-397.486	-394.931	68.764
400	105.855	235.422	208.690	10.693	-422.002	-393.180	31.344
500	106.274	239.088	216.490	21.299	-486.315	-379.800	39.677
600	106.692	278.504	225.255	31.949	-483.987	-358.717	31.229
700	106.901	294.966	234.068	42.629	-481.726	-338.018	25.223
800	107.110	309.254	242.593	53.329	-479.544	-317.638	20.740
900	107.320	321.883	250.715	64.051	-477.454	-297.526	17.268
1000	107.445	333.197	258.407	74.790	-475.474	-277.642	14.503
1100	107.529	343.442	265.679	85.539	-473.620	-257.949	12.249
1200	107.612	352.802	272.555	96.296	-471.814	-238.198	10.368
1300	107.696	361.419	279.064	107.062	-470.050	-218.500	8.779
1400	107.738	369.401	285.235	117.833	-471.470	-198.961	7.423
1500	107.780	376.836	291.097	128.609	-469.548	-179.564	6.253
1600	107.822	383.793	296.675	139.389	-467.761	-160.291	5.233
1700	107.864	390.331	301.994	150.174	-466.131	-141.124	4.336
1800	107.905	396.498	307.074	160.962	-464.679	-122.049	3.542
1900	107.947	402.333	311.936	171.755	-463.423	-103.050	2.833
2000	107.989	407.871	316.595	182.551	-462.373	-84.111	2.197

Enthalpy Reference Temperature = T<sub>r</sub> = 298.15 K

Standard State Pressure = P<sup>o</sup> = 0.1 MPa

PREVIOUS: June 1962

CURRENT: June 1964

Zirconium Iodide (ZrI<sub>3</sub>)I<sub>3</sub>Zr<sub>1</sub>(g)

Zirconium Iodide (ZrI<sub>3</sub>)

IDEAL GAS

M<sub>r</sub> = 471.9335 Zirconium Iodide (ZrI<sub>3</sub>)

I<sub>3</sub>ZrI<sub>3</sub>(g)

S°(298.15 K) = [397.776] J·K<sup>-1</sup>·mol<sup>-1</sup>      ΔH<sup>o</sup>(0 K) = [-216.860] kJ·mol<sup>-1</sup>      log K<sub>r</sub> INFINITE  
 ΔH<sup>o</sup>(298.15 K) = [-221.752] kJ·mol<sup>-1</sup>      ΔH<sup>o</sup>(298.15 K) = [-221.752] kJ·mol<sup>-1</sup>      ΔG<sup>o</sup> INFINITE

Vibrational Frequencies and Degeneracies

- v<sub>1</sub>, cm<sup>-1</sup>
- [195](1)
- [88](1)
- [220](2)
- [65](2)

Ground State Quantum Weight: [2]      σ = [3]  
 Point Group: [C<sub>3v</sub>]  
 Bond Distance: Zr-I = [2.59] Å  
 Bond Angle: I-Zr-I = [101]°  
 Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [1.155142 × 10<sup>-110</sup>] g<sup>3</sup>·cm<sup>6</sup>

Enthalpy of Formation

The enthalpies of formation, from the gaseous atoms, of the gaseous zirconium tetrahalides were computed from data issued in these tables. The zirconium-halide bond energy, taken as 1/4 of this enthalpy of formation, was found to be linear with internuclear separation. From the zirconium-triiodide and tetraiodide, it was found that the bond energy of the triiodide was around 7 kcal·mol<sup>-1</sup> greater than that for titanium trichloride. This amount was added to the bond energy of zirconium trichloride to get that of zirconium trichloride which, when used with its estimated internuclear distance, was found to lie almost exactly on the bond energy versus internuclear distance curve for the tetrahalides. The bond energy for each of the gaseous trihalides of zirconium was determined from this curve and their estimated bond distances.

For zirconium triiodide, the enthalpy of formation from the gaseous atoms was -275 kcal·mol<sup>-1</sup> and from the elements in their standard state, -53 kcal·mol<sup>-1</sup>.

Heat Capacity and Entropy

The measured internuclear distances for the triiodides of phosphorus, arsenic, and antimony were plotted as a function of the atomic weight of these elements and a smooth curve was drawn through the points. The bond distance in ZrI<sub>3</sub> was taken from this plot. The bond angle was assumed to be 101°. The principal moments of inertia are: I<sub>A</sub> = I<sub>B</sub> = 185.2317 × 10<sup>-39</sup> and I<sub>C</sub> = 336.6703 × 10<sup>-39</sup> g·cm<sup>2</sup>.

Force constants for ZrI<sub>3</sub> were estimated from those of the triiodides of phosphorus and arsenic. These were used in a valence force field calculation giving ν<sub>1</sub> = 195, ν<sub>2</sub> = 88, ν<sub>3</sub> = 181, and ν<sub>4</sub> = 65 cm<sup>-1</sup> for the fluorides and chlorides of P, As, and Sb, ν<sub>1</sub> is greater than ν<sub>2</sub> but there appears to be a reversal as one goes to the bromides and iodides with ν<sub>3</sub> becoming greater than ν<sub>1</sub>. An empirical correlation procedure for ZrI<sub>3</sub> gave ν<sub>1</sub> = 195, ν<sub>2</sub> = 90, ν<sub>3</sub> = 220, and ν<sub>4</sub> = 65 cm<sup>-1</sup> in which ν<sub>3</sub> > ν<sub>1</sub>. Since ν<sub>3</sub> > ν<sub>1</sub> for PI<sub>3</sub> and AsI<sub>3</sub>, the correlation value for ν<sub>3</sub> was used to represent this frequency in ZrI<sub>3</sub>.

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - [H <sup>o</sup> (T)]	ΔH <sup>o</sup>	log K <sub>r</sub>
0	0	INFINITE	INFINITE	-216.860	INFINITE
100	68.161	314.735	-20.403	-217.195	-218.115
200	78.257	363.960	-15.277	-217.195	-218.115
250	79.902	383.617	-8.871	-219.240	-219.240
298.15	80.820	397.776	0	-220.539	-220.539
300	80.847	398.276	0.150	-221.752	-221.752
350	81.436	410.786	4.208	-221.800	-221.800
400	81.826	421.688	8.290	-222.231	-222.231
450	82.097	431.342	12.388	-223.046	-223.046
500	82.292	440.002	16.498	-224.281	-224.281
600	82.549	455.031	24.741	-227.563	-227.563
700	82.766	467.768	33.005	-232.875	-232.875
800	82.808	478.819	41.281	-240.610	-240.610
900	82.878	488.577	49.565	-250.309	-250.309
1000	82.928	497.312	57.856	-262.962	-262.962
1100	82.966	505.218	66.151	-278.580	-278.580
1200	82.994	512.438	74.449	-307.373	-307.373
1300	83.016	519.082	82.749	-352.085	-352.085
1400	83.034	525.235	91.052	-418.181	-418.181
1500	83.048	530.964	99.356	-507.074	-507.074
1600	83.060	536.324	107.661	-620.340	-620.340
1700	83.069	541.360	115.968	-760.307	-760.307
1800	83.077	546.108	124.275	-939.307	-939.307
1900	83.084	550.600	132.583	-1160.866	-1160.866
2000	83.090	554.862	140.892	-1438.305	-1438.305
2100	83.095	558.916	149.201	-1786.961	-1786.961
2200	83.099	562.782	157.511	-2234.687	-2234.687
2300	83.103	566.476	165.821	-2832.245	-2832.245
2400	83.107	570.013	174.131	-3539.672	-3539.672
2500	83.109	573.405	182.442	-4400.880	-4400.880
2600	83.112	576.665	190.753	-5472.627	-5472.627
2700	83.114	579.802	199.065	-6802.220	-6802.220
2800	83.116	582.824	207.376	-8449.977	-8449.977
2900	83.118	585.741	215.688	-10479.556	-10479.556
3000	83.120	588.559	224.000	-12968.183	-12968.183
3100	83.122	591.284	232.312	-16089.645	-16089.645
3200	83.123	593.933	240.624	-19999.291	-19999.291
3300	83.124	596.481	248.937	-25862.645	-25862.645
3400	83.125	598.963	257.249	-34077.141	-34077.141
3500	83.126	601.372	265.562	-45222.222	-45222.222
3600	83.127	603.714	273.874	-60067.979	-60067.979
3700	83.128	605.992	282.187	-79492.871	-79492.871
3800	83.129	608.209	290.500	-104424.182	-104424.182
3900	83.130	610.368	298.813	-136943.474	-136943.474
4000	83.131	612.473	307.126	-178605.160	-178605.160
4100	83.131	614.525	315.439	-231730.000	-231730.000
4200	83.132	616.529	323.752	-300199.147	-300199.147
4300	83.132	618.485	332.065	-388813.353	-388813.353
4400	83.133	620.396	340.379	-494862.126	-494862.126
4500	83.133	622.264	348.692	-624835.102	-624835.102
4600	83.134	624.091	357.005	-785151.917	-785151.917
4700	83.134	625.879	365.318	-984689.439	-984689.439
4800	83.135	627.650	373.632	-1231589.598	-1231589.598
4900	83.135	629.344	381.946	-1536894.383	-1536894.383
5000	83.135	631.023	390.259	-1912222.176	-1912222.176
5100	83.136	632.670	398.573	-2370612.278	-2370612.278
5200	83.136	634.284	406.886	-2928248.215	-2928248.215
5300	83.136	635.868	415.200	-3601937.401	-3601937.401
5400	83.137	637.422	423.514	-4409975.577	-4409975.577
5500	83.137	638.947	431.827	-5369914.767	-5369914.767
5600	83.137	640.445	440.141	-6509915.913	-6509915.913
5700	83.137	641.917	448.455	-7869929.127	-7869929.127
5800	83.138	643.362	456.769	-9499955.376	-9499955.376
5900	83.138	644.784	465.082	-11469995.596	-11469995.596
6000	83.138	646.181	473.396	-13869985.865	-13869985.865

PREVIOUS: June 1964 (1 atm)

CURRENT: June 1964 (1 bar)

Zirconium Iodide (ZrI<sub>3</sub>)

I<sub>3</sub>ZrI<sub>3</sub>(g)

## CRYSTAL

Molybdenum Iodide (MoI<sub>4</sub>)M<sub>r</sub> = 603.5580Molybdenum Iodide (MoI<sub>4</sub>)I<sub>4</sub>Mo<sub>1</sub>(cr)

$S^{\circ}(298.15 \text{ K}) = [266.061 \pm 16.7] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$   
 $T_{\text{dem}} = [293] \text{ K}$   
 $\Delta_f H^{\circ}(0 \text{ K}) = \text{Unknown}$   
 $\Delta_f H^{\circ}(298.15 \text{ K}) = [-123.010 \pm 8.4] \text{ kJ} \cdot \text{mol}^{-1}$

## Enthalpy of Formation

We adopt the  $\Delta_f H^{\circ}(298.15 \text{ K})$  value estimated by Brewer.<sup>1</sup> This value predicts that MoI<sub>4</sub>(cr) is unstable with respect to MoI<sub>3</sub>(cr) at temperatures above 293 K.<sup>1</sup> This is consistent with the observations of Lewis *et al.*<sup>2</sup> who found that only the crystalline triiodide is formed by heating pure Mo metal in excess iodine in a sealed tube to 573 K. Brewer's estimated value is given as  $\Delta_f H^{\circ}(298.15 \text{ K})/R = -14800 \pm 1000 \text{ K}$ . The assigned uncertainty ( $\pm 2 \text{ kcal} \cdot \text{mol}^{-1}$ ) is determined from the product  $1000 \times R$  which has been rounded to the nearest kcal·mol<sup>-1</sup>.

## Heat Capacity and Entropy

The values of  $C_p^{\circ}$  and  $S^{\circ}$  at 298.15 K are estimates reported by Brewer.<sup>1</sup> We assume a constant  $C_p^{\circ}$  of 32.79 cal·K<sup>-1</sup>·mol<sup>-1</sup> over the temperature range 298–600 K. The value of  $S^{\circ}(298.15 \text{ K})/R$  reported by Brewer<sup>1</sup> is treated in a manner similar to that for the enthalpy of formation.

## Phase Data

The preparation of MoI<sub>4</sub>(cr) has been reported by Guichard<sup>3</sup> but the sample was impure. The stability range of the tetraiodide appears to be small based on the observations of Lewis *et al.*<sup>2</sup> who found that MoI<sub>4</sub> could not be formed by heating Mo in excess iodine in a sealed tube to 573 K.

## Decomposition Data

Brewer<sup>1</sup> estimated a  $T_{\text{dem}}$  of 293 K from free energy data for the dissociation reaction  $\text{MoI}_4(\text{cr}) = \text{MoI}_3(\text{cr}) + 0.5 \text{I}_2(\text{cr})$ . We adopt this value since  $T_{\text{dem}}$  appears to lie outside the temperature range selected for our MoI<sub>4</sub>(cr) phase table.

## References

1. L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, personal communication, September 29, 1978, preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria.
2. J. Lewis, D. J. Machin, R. S. Nyholm, P. Pauling, and P. W. Smith, Chemistry and Industry, 1960, 259 (1960).
3. M. Guichard, Annales de Chimie et de Physique, 23, 498 (1901).

T/K	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = p° = 0.1 MPa	
	C <sub>p</sub> <sup>o</sup>	S° - (G° - H°(T))/T	H° - H°(T)	Δ <sub>f</sub> G°
0				
100				
200				
298.15	137.193	266.061	0	-124.552
300	137.193	266.909	0.254	-124.561
400	137.193	306.377	13.973	-123.992
500	137.193	336.991	27.692	-106.063
600	137.193	362.004	41.412	-81.970
				log K <sub>r</sub>
				21.821
				21.688
				16.192
				11.290
				7.136

PREVIOUS.

CURRENT September 1978

Molybdenum Iodide (MoI<sub>4</sub>)I<sub>4</sub>Mo<sub>1</sub>(cr)



Molybdenum Iodide (Mol.)

IDEAL GAS

M<sub>r</sub> = 603.5580 Molybdenum Iodide (Mol.)

I<sub>4</sub>Mo<sub>1</sub>(g)

S<sup>0</sup>(298.15 K) = [452.812 ± 12.6] J·K<sup>-1</sup>·mol<sup>-1</sup>      Δ<sub>f</sub>H<sup>0</sup>(0 K) = [129.32 ± 41.8] kJ·mol<sup>-1</sup>      Δ<sub>f</sub>H<sup>0</sup>(298.15 K) = [124.68 ± 41.8] kJ·mol<sup>-1</sup>

Electronic Levels and Quantum Weights	
ε, cm <sup>-1</sup>	g <sub>e</sub>
0	[3]
[15000]	[11]
[20000]	[9]
Vibrational Frequencies and Degeneracies	
ν, cm <sup>-1</sup>	ν, cm <sup>-1</sup>
[150](1)	[240](3)
[50](2)	[60](3)

Point Group: [Td]  
 Bond Distance: Mo-I = [2.66] Å  
 Bond Angle: I-Mo-I = [109°28']  
 Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [6.286307 × 10<sup>-110</sup>] g<sup>3</sup>·cm<sup>6</sup>  
 σ = [12]

Enthalpy of Formation

We adopt the Δ<sub>f</sub>H<sup>0</sup>(298.15 K) value estimated by Brewer.<sup>1</sup> This estimated value is consistent with the low volatility of metallic molybdenum in iodine vapor reported by Schafer *et al.*<sup>2</sup> Brewer's estimated value is given as Δ<sub>f</sub>H<sup>0</sup>(298.15 K) = 15000 ± 5000 K. The assigned uncertainty (10 kcal·mol<sup>-1</sup>) is determined from the product 5000xR, which has been rounded to the nearest kcal·mol<sup>-1</sup>. Combining the Δ<sub>f</sub>H<sup>0</sup>(0 K) value with JANAF data on Mo(g) and I(g), we calculate a heat of atomization Δ<sub>at</sub>H<sup>0</sup>(0 K) of 228.7 ± 11 kcal·mol<sup>-1</sup> and a mean bond dissociation energy Δ<sub>b</sub>H<sup>0</sup>(0 K) = 57.2 ± 2.5 kcal·mol<sup>-1</sup>.

Heat Capacity and Entropy

The vibrational frequencies and molecular structural data are estimates taken from Brewer.<sup>1</sup> The principal moments of inertia are I<sub>A</sub> = I<sub>B</sub> = I<sub>C</sub> = 397.6172 × 10<sup>-99</sup> g·cm<sup>2</sup>. The electronic levels and degeneracies are those predicted by Brewer for MoF<sub>4</sub>(g) from crystal field theory. The upper levels contribute 0.23 cal·K<sup>-1</sup>·mol<sup>-1</sup> to the Gibbs energy function at 6000 K.

References

- L. Brewer, Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley; personal communication, September 29, 1978, preliminary draft of review to be submitted for publication in Atomic Energy Review, International Atomic Energy Agency, Vienna, Austria.
- H. Schafer, T. Grofe, and M. Trenkel, J. Solid State Chem. 8, 14 (1973).

<sup>1</sup>JANAF Thermochemical Tables: Mo(g), 3-31-78, I(g), 6-30-74.

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>0</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>0</sup>	S <sup>0</sup> - [C <sub>p</sub> <sup>0</sup> - H <sup>0</sup> (T <sub>r</sub> )]/T <sub>r</sub>	H <sup>0</sup> - H <sup>0</sup> (T <sub>r</sub> )	Δ <sub>f</sub> G <sup>0</sup>	
0	0	INFINITE	-26.344	129.320	INFINITE
100	88.395	345.225	-19.796	129.277	-56.233
200	101.392	411.558	-10.152	127.214	-22.665
250	103.615	434.446	-5.022	125.971	-16.049
298.15	104.869	452.812	0	124.683	-11.819
300	104.906	453.461	0.194	124.631	-11.684
350	105.716	469.698	5.461	123.061	-8.602
400	106.254	483.851	10.761	119.467	-6.464
450	106.629	496.389	16.084	115.458	-5.194
500	106.901	507.639	21.422	111.186	-4.018
600	107.258	527.163	32.132	105.716	-2.993
700	107.476	543.715	42.869	100.194	-2.167
800	107.618	558.076	49.104	94.632	-1.515
900	107.716	570.758	49.912	89.166	-1.002
1000	107.786	582.111	50.694	83.855	-0.643
1100	107.838	592.386	51.452	78.683	-0.385
1200	107.878	601.771	52.159	73.653	-0.200
1300	107.909	610.407	52.797	68.760	-0.084
1400	107.935	618.405	53.389	64.000	-0.034
1500	107.957	625.853	53.979	59.466	-0.011
1600	107.977	632.821	54.579	55.147	0.000
1700	107.998	639.367	55.171	51.036	0.000
1800	108.022	645.541	55.751	47.126	0.000
1900	108.051	651.382	56.309	43.500	0.000
2000	108.088	656.925	56.837	40.153	0.000
2100	108.135	662.200	57.333	37.070	0.000
2200	108.195	667.232	57.795	34.245	0.000
2300	108.270	672.043	58.318	31.666	0.000
2400	108.363	676.653	58.800	29.320	0.000
2500	108.476	681.079	59.241	27.199	0.000
2600	108.611	685.336	59.639	25.281	0.000
2700	108.768	689.438	59.975	23.552	0.000
2800	108.936	693.396	60.252	22.000	0.000
2900	109.116	697.223	60.471	20.610	0.000
3000	109.308	700.928	60.630	19.370	0.000
3100	109.514	704.518	60.735	18.270	0.000
3200	109.724	708.004	60.786	17.300	0.000
3300	110.228	711.391	60.792	16.450	0.000
3400	110.554	714.686	60.758	15.710	0.000
3500	110.901	717.896	60.688	15.070	0.000
3600	111.267	721.025	60.583	14.520	0.000
3700	111.650	724.079	60.448	14.050	0.000
3800	112.049	727.062	60.288	13.650	0.000
3900	112.460	729.978	60.108	13.310	0.000
4000	112.882	732.830	60.000	13.020	0.000
4100	113.313	735.623	60.000	12.780	0.000
4200	113.749	738.359	60.000	12.580	0.000
4300	114.189	741.040	60.000	12.420	0.000
4400	114.630	743.671	60.000	12.290	0.000
4500	115.071	746.252	60.000	12.190	0.000
4600	115.508	748.786	60.000	12.110	0.000
4700	115.940	751.274	60.000	12.050	0.000
4800	116.365	753.720	60.000	12.000	0.000
4900	116.780	756.123	60.000	11.960	0.000
5000	117.185	758.487	60.000	11.930	0.000
5100	117.578	760.811	60.000	11.910	0.000
5200	117.957	763.098	60.000	11.900	0.000
5300	118.321	765.348	60.000	11.900	0.000
5400	118.669	767.563	60.000	11.910	0.000
5500	119.000	769.744	60.000	11.930	0.000
5600	119.314	771.891	60.000	11.960	0.000
5700	119.609	774.005	60.000	12.000	0.000
5800	119.886	776.088	60.000	12.050	0.000
5900	120.144	778.140	60.000	12.110	0.000
6000	120.383	780.161	60.000	12.180	0.000

PREVIOUS: September 1978 (1 atm)

CURRENT: September 1978 (1 bar)

Molybdenum Iodide (Mol.)

I<sub>4</sub>Mo<sub>1</sub>(g)

I<sub>4</sub>Pb<sub>4</sub>(g)Lead Iodide (PbI<sub>2</sub>)M<sub>r</sub> = 714.8180

$$\Delta_f H^\circ(0 \text{ K}) = [-218.82 \pm 83.7] \text{ kJ mol}^{-1}$$

$$\Delta_f H^\circ(298.15 \text{ K}) = [-224.47 \pm 83.7] \text{ kJ mol}^{-1}$$

$$S^\circ(298.15 \text{ K}) = [466.266 \pm 12.6] \text{ J K}^{-1} \text{ mol}^{-1}$$

Vibrational Frequencies and Degeneracies

ν<sub>b</sub>, cm<sup>-1</sup>

[137](1)  
[37](2)  
[168](3)  
[48](3)

Ground State Quantum Weight: [1]

Point Group: [T<sub>d</sub>]

Bond Distance: Pb-I = [2.77] Å

Bond Angle: I-Pb-I = [109°28']

Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [8.016506 × 10<sup>-109</sup>] g<sup>3</sup> cm<sup>6</sup>

σ = [12]

**Enthalpy of Formation**

The adopted  $\Delta_f H^\circ(0 \text{ K}) = -52.3 \pm 20 \text{ kcal mol}^{-1}$  is derived from the atomization energy for the process  $\text{PbI}_4(\text{g}) = \text{Pb}(\text{g}) + 4 \text{ I}(\text{g})$ .  $\Delta_f H^\circ(0 \text{ K}) = 8.75 \text{ eV}$  is estimated from an intercomparison of the lead mono-, di-, and tetra-halides.<sup>1</sup> This adopted value for  $\text{PbI}_4(\text{g})$  is greater than the  $\Delta_f H^\circ(0 \text{ K})$  value for  $\text{PbI}(\text{g})$  by a factor of 2.04. The auxiliary values  $\Delta_f H^\circ(\text{Pb}, \text{g}, 0 \text{ K}) = 46.9 \text{ kcal mol}^{-1}$  and  $\Delta_f H^\circ(\text{I}, \text{g}, 0 \text{ K}) = 25.633 \text{ kcal mol}^{-1}$  are used.  $\Delta_f H^\circ(\text{PbI}_4, \text{g}, 298.15 \text{ K}) = -53.6 \pm 20 \text{ kcal mol}^{-1}$  is calculated from  $\Delta_f H^\circ(0 \text{ K})$ .

**Heat Capacity and Entropy**

The molecular constants and vibrational frequencies are those calculated by Aleksandrovskaya *et al.*<sup>2</sup> Later works<sup>4, 5</sup> mistakenly cite this work as observed data.

The principal moments of inertia are:  $I_A = I_B = I_C = 431.1831 \times 10^{-39} \text{ g cm}^2$ .

**References**

- <sup>1</sup>JANAF Thermochemical Tables:  $\text{PbF}(\text{g})$ ,  $\text{PbF}_2(\text{g})$ ,  $\text{PbF}_3(\text{g})$ ,  $\text{PbBr}(\text{g})$ ,  $\text{PbBr}_2(\text{g})$ ,  $\text{PbI}(\text{g})$  and  $\text{PbI}_2(\text{g})$ ,  $\text{PbCl}(\text{g})$  and  $\text{PbCl}_2(\text{g})$ , 6-30-73,  $\text{Pb}(\text{g})$ , 3-31-62, [g], 12-31-61.
- <sup>2</sup>A. M. Aleksandrovskaya, I. V. Rigma, and I. N. Godnev, *Optics and Spectrosc.* **7**, 495 (1959).
- <sup>3</sup>G. Nagargan, *Bull. Soc. Chim. Belges*, **71**, 119 (1962).
- <sup>4</sup>M. Radhakrishnan, *Indian J. Pure Appl. Phys.* **1**, 402 (1963).
- <sup>5</sup>S. P. Singh, *Ladhev, Part A*, **7**, 185 (1969).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> ° - H <sub>f</sub> °(T <sub>r</sub> )]/T	H <sub>f</sub> ° - H <sub>f</sub> °(T <sub>r</sub> )	Δ <sub>f</sub> H <sup>o</sup>	
0	0	0	INFINITE	INFINITE	INFINITE
100	95.214	354.506	559.058	-218.820	124.885
200	104.275	424.175	475.941	-219.084	124.885
250	105.593	447.600	468.013	-221.799	67.330
298.15	106.313	466.266	466.266	-224.467	55.713
300	106.334	466.924	466.268	-224.522	48.164
350	106.790	483.352	467.565	-226.170	47.921
400	107.089	497.633	470.450	-228.518	42.318
450	107.259	510.259	474.185	-229.851	37.940
500	107.445	521.572	478.368	-229.659	34.141
600	107.640	541.180	487.252	-229.961	30.261
700	107.758	557.782	496.172	-229.971	24.199
800	107.835	572.177	504.793	-229.558	19.811
900	107.888	584.881	513.000	-228.096	15.270
1000	107.926	596.250	520.766	-226.333	11.927
1100	107.954	606.538	528.103	-225.988	10.256
1200	107.975	615.932	535.037	-225.664	8.865
1300	107.991	624.576	541.596	-225.360	7.689
1400	108.005	632.579	547.813	-225.070	6.681
1500	108.015	640.031	553.715	-224.790	5.808
1600	108.024	647.002	559.330	-224.512	5.044
1700	108.031	653.552	564.682	-224.228	4.370
1800	108.037	659.727	569.792	-223.931	3.770
1900	108.042	665.568	574.681	-223.623	3.233
2000	108.047	671.110	579.365	-223.307	2.749
2100	108.051	676.382	583.860	-222.985	2.333
2200	108.054	681.408	588.101	-222.658	1.933
2300	108.057	686.212	592.339	-222.326	1.546
2400	108.059	690.810	596.347	-221.991	1.178
2500	108.061	695.222	600.215	-221.654	0.831
2600	108.063	699.460	603.951	-221.316	0.507
2700	108.065	703.538	607.564	-220.974	0.212
2800	108.067	707.468	611.062	-220.628	0.811
2900	108.068	711.261	614.452	-220.278	1.182
3000	108.069	714.924	617.741	-219.924	1.528
3100	108.070	718.468	620.933	-219.566	1.852
3200	108.071	721.899	624.035	-219.205	2.156
3300	108.072	725.225	627.051	-218.841	2.442
3400	108.073	728.451	629.986	-218.473	2.711
3500	108.074	731.584	632.845	-218.102	2.965
3600	108.075	734.628	635.630	-217.728	3.205
3700	108.076	737.589	638.346	-217.351	3.433
3800	108.077	740.472	640.985	-216.971	3.648
3900	108.077	743.279	643.582	-216.588	3.853
4000	108.077	746.015	646.109	-216.202	4.047
4100	108.078	748.684	648.578	-215.812	4.232
4200	108.078	751.288	650.993	-215.419	4.409
4300	108.079	753.831	653.355	-215.024	4.577
4400	108.079	756.316	655.667	-214.627	4.737
4500	108.079	758.745	657.931	-214.228	4.890
4600	108.080	761.120	660.148	-213.827	5.037
4700	108.080	763.445	662.322	-213.424	5.177
4800	108.080	765.720	664.452	-213.019	5.311
4900	108.081	767.949	666.542	-212.612	5.440
5000	108.081	770.132	668.592	-212.203	5.564
5100	108.081	772.273	670.604	-211.792	5.682
5200	108.081	774.371	672.579	-211.379	5.796
5300	108.082	776.430	674.519	-210.964	5.905
5400	108.082	778.450	676.425	-210.548	6.010
5500	108.082	780.434	678.298	-210.131	6.111
5600	108.082	782.381	680.140	-209.712	6.208
5700	108.082	784.294	681.950	-209.292	6.302
5800	108.083	786.174	683.731	-208.871	6.392
5900	108.083	788.022	685.483	-208.449	6.479
6000	108.083	789.838	687.207	-208.026	6.563

PREVIOUS: December 1973 (1 atm)

CURRENT: December 1973 (1 bar)

Lead Iodide (PbI<sub>2</sub>)I<sub>4</sub>Pb<sub>4</sub>(g)

Tetraiodosilane (SiI<sub>4</sub>)

CRYSTAL

M<sub>r</sub> = 535.7035

Tetraiodosilane (SiI<sub>4</sub>)

I<sub>4</sub>Si<sub>1</sub>(cr)

S°(298.15 K) = [258.153 ± 3.3] J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>sub</sub> = 393.65 ± 3.0 K

ΔH<sup>o</sup>(0 K) = Unknown  
 ΔH<sup>o</sup>(298.15 K) = -189.54 ± 16.7 kJ·mol<sup>-1</sup>  
 Δ<sub>int</sub> H° = 19.665 ± 2.1 kJ·mol<sup>-1</sup>

Enthalpy of Formation

Schafer and Heine<sup>1</sup> measured the enthalpies of solution of Si(cr) and SiI<sub>4</sub>(cr) in an HF solution containing AgF. For the overall reaction SiI<sub>4</sub>(cr) + 4Ag(cr) = Si(cr) + 4AgI(cr), they reported ΔH°(298.15 K) = -13.80 ± 0.44 kcal·mol<sup>-1</sup>. Using auxiliary data for AgI<sup>2</sup> we calculate ΔH°(298.15 K) = 45.3 kcal·mol<sup>-1</sup> for SiI<sub>4</sub>(cr). We adopt this value and assign an uncertainty of ±4.0 kcal·mol<sup>-1</sup> due to the overall inconsistency in the SiI<sub>4</sub> thermochemical data. Refer to the SiI<sub>4</sub>(g) table for more details.

Wolf<sup>3</sup> studied the enthalpies of solution of SiI<sub>4</sub>(cr) and Na<sub>2</sub>SiO<sub>3</sub>(cr) in caustic solution. The net reaction of interest SiI<sub>4</sub>(cr) + 6NaOH(cr) = Na<sub>2</sub>SiO<sub>3</sub>(cr) + 4NaI(cr) + 3H<sub>2</sub>O(l) yielded an enthalpy of reaction of ΔH°(298.15 K) = -191.5 ± 1.5 kcal·mol<sup>-1</sup> based on the appropriate combination of results from five solution studies. Using current auxiliary data,<sup>4,5</sup> we calculate ΔH°(298.15 K) = -51.0 kcal·mol<sup>-1</sup> for SiI<sub>4</sub>(cr). This data is suspect due to uncertainties in how Wolf converted his data from Na<sub>2</sub>SiO<sub>3</sub>(calorimetric solution) to Na<sub>2</sub>SiO<sub>3</sub>(cr).

Heat Capacity and Entropy

The adopted heat capacity values are from the study of Kurosawa, *et al.*<sup>6</sup> The data was obtained from an adiabatic calorimeter of a type used for specific heat measurements and differential thermal analysis. Similar studies on Cr(cr) and Si(cr) would suggest uncertainties of the order of 3% near room temperature and 0-10% at 600-70 K.

There is no low temperature heat capacity data for T < 298.15 K. The entropy at 298.15 K is chosen from a consideration of the sublimation and vaporization data. Refer to the SiI<sub>4</sub>(g) table for additional information. However, the discrepancies in the various vapor pressure studies are such that a precise estimate of the entropy is not possible.

Fusion Data

Kurosawa *et al.*<sup>6</sup> using differential thermal analysis (DTA) techniques, determined Δ<sub>sub</sub>H° = 4.7 kcal·mol<sup>-1</sup>, an average of eight measurements with a standard deviation of 0.08 kcal·mol<sup>-1</sup>. The same study reported T<sub>sub</sub> = 120.5°C as determined from the cooling curve. McCarty *et al.*<sup>7</sup> reported T<sub>sub</sub> = 123.68 ± 0.06°C for 99.998% (mole) pure SiI<sub>4</sub>. Other studies have listed melting points in the range 120-127°C as reported by Kurosawa *et al.*<sup>6</sup> The sublimation and vaporization studies of Bartsch and Wolf<sup>8</sup> suggest a melting point of 123.5°C and a heat of melting of 4.1 ± 0.6 kcal·mol<sup>-1</sup>. Due to the short temperature range of measurement in each condensed phase, precise melting data is not expected. In general, the vapor pressure studies, as discussed in the SiI<sub>4</sub>(g) table<sup>6</sup> show poor agreement in the vicinity of T<sub>sub</sub>.

We adopt T<sub>sub</sub> = 120.5°C and Δ<sub>sub</sub>H° = 4.7 kcal·mol<sup>-1</sup> as derived from Kurosawa *et al.*<sup>6</sup> We assign respective uncertainties of ±3.0 K and 0.5 kcal·mol<sup>-1</sup> due to the variances among the various studies.

Sublimation Data

The enthalpy of sublimation, Δ<sub>sub</sub>H°(298.15 K), is the difference between the Δ<sub>sub</sub>H°(298.15 K) values for SiI<sub>4</sub>(g) and SiI<sub>4</sub>(cr). Three sublimation studies are summarized in the SiI<sub>4</sub>(g) table.

References

- <sup>1</sup>H. Schafer and H. Heine, *Z. anorg. Chem.* **332**, 25 (1964).
- <sup>2</sup>U. S. Nat. Bur. Stand. Tech. Note 270-4, 141 pp. (1969).
- <sup>3</sup>E. Wolf, *Z. Chem.* **7**, 283 (1967).
- <sup>4</sup>J. D. Cox, ICSU CODATA Task Group on Key Values for Thermodynamics, *J. Chem. Thermodyn.* **4**, 331 (1972).
- <sup>5</sup>JANAF Thermochemical Tables: NaI(cr), 9-30-63; NaOH(cr), 12-31-70; Na<sub>2</sub>SiO<sub>3</sub>(cr), 9-30-67; SiCl<sub>4</sub>(g), 12-31-70; SiI<sub>4</sub>(cr), 6-30-76.
- <sup>6</sup>T. Kurosawa, R. Hasegawa, and T. Yagihashi, *Trans. Japan Inst. Metals.* **6**, 229 (1965); *Trans. Natl. Res. Inst. Metals.* (Tokyo) **7**, 222 (1965).
- <sup>7</sup>L. V. McCarty, L. C. Landauer, and J. M. Binkowski, *J. Chem. Eng. Data* **5**, 365-6 (1960).
- <sup>8</sup>K. Bartsch and E. Wolf, *Z. anorg. allg. Chem.* **383**, 66 (1971).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K			Standard State Pressure = p° = 0.1 MPa		
	C <sub>p</sub> <sup>o</sup>	S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	Δ <sub>sub</sub> H°	Δ <sub>sub</sub> G°	log K <sub>r</sub>
0						
100						
200						
298.15	108.035	258.153	0.	-189.535	-191.637	33.574
300	108.198	258.822	0.200	-189.574	-191.650	33.369
393.650	116.388	289.279	10.716	---	CRYSTAL <---> LIQUID	---
400	116.943	291.146	262.503	-223.715	-190.911	24.930
500	125.687	318.180	271.003	-310.254	-174.369	18.216

PREVIOUS.

CURRENT: June 1976

Tetraiodosilane (SiI<sub>4</sub>)

I<sub>4</sub>Si<sub>1</sub>(cr)

Tetraiodosilane (SiI<sub>4</sub>)

## LIQUID

M<sub>r</sub> = 535.7035Tetraiodosilane (SiI<sub>4</sub>)I<sub>4</sub>Si<sub>1</sub>(l)

S°(298.15 K) = [294.309] J K<sup>-1</sup> mol<sup>-1</sup>  
 T<sub>fm</sub> = 393.65 ± 3.0 K

## Enthalpy of Formation

$\Delta_f H^\circ(\text{SiI}_4, l, 298.15 \text{ K})$  is calculated from that of the crystal by adding the enthalpy of melting,  $\Delta_{\text{melt}} H^\circ$ , and the difference in enthalpy,  $H^\circ(393.65 \text{ K}) - H^\circ(298.15 \text{ K})$ , between the crystal and liquid.

## Heat Capacity and Entropy

Kurosawa *et al.*<sup>1</sup> measured the heat capacity of SiI<sub>4</sub> from the melting point (unspecified). No data was presented but rather smoothed results were represented by an equation, linear in  $T$ . This equation is extrapolated to 700 K and to 298.15 K.  $S^\circ(298.15 \text{ K})$  is calculated in a manner analogous to that used for  $\Delta_f H^\circ(298.15 \text{ K})$ .

## Vaporization Data

$T_{\text{vap}} = -576 \text{ K}$  is calculated as that temperature at which the fugacity is one atmosphere for the process  $\text{SiI}_4(l) = \text{SiI}_4(g)$ .  $\Delta_{\text{vap}} H^\circ$  is calculated as the difference between the  $\Delta_f H^\circ$  values for the ideal gas and the liquid at  $T_{\text{vap}}$ . The vaporization studies near  $T_{\text{vap}}$  are discussed in the SiI<sub>4</sub>(g) table; they yielded normal boiling points ( $p = 760 \text{ mm Hg}$ ) of 574.7 K and 573.7 K. The normal boiling point should be slightly lower than our calculated  $T_{\text{vap}}$ , which corresponds to  $f = 760 \text{ mm Hg}$ .

## References

- <sup>1</sup>T. Kurosawa, R. Hasegawa, and T. Yagihashi, *Trans. Japan Inst. Metals*, **6**, 229 (1965); *Trans. Natl. Res. Metals (Toyko)* **7**, 222 (1965).
- <sup>2</sup>H. C. Andersen and L. H. Belfz, *J. Amer. Chem. Soc.* **75**, 4828 (1953).
- <sup>3</sup>K. Uchimura, T. Takuma, M. Yuizumi and T. Kumugi, *Denki Kagaku* **5**, 876 (1967).

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
		S° - (G° - H°(T <sub>r</sub> ))/T	H° - H°(T <sub>r</sub> )	Δ <sub>r</sub> H°	Δ <sub>r</sub> G°	
0						
100						
200						
298.15	159.800	294.309	294.309	0.	-174.603	-187.485
300	159.875	295.298	294.312	0.296	-174.546	-187.565
393.650	163.744	339.234	299.988	15.449	---	---
400	164.004	341.856	300.632	16.490	---	---
500	168.134	378.897	312.703	33.097	---	---
600	172.264	409.916	326.389	50.117	---	---
700	176.393	436.781	340.282	67.549	---	---

CRYSTAL <---> LIQUID

PREVIOUS: June 1976

CURRENT: December 1977

Tetraiodosilane (SiI<sub>4</sub>)I<sub>4</sub>Si<sub>1</sub>(l)

Tetraiodosilane (SiI<sub>4</sub>)

M<sub>r</sub> = 535.7035 Tetraiodosilane (SiI<sub>4</sub>)

CRYSTAL-LIQUID

I<sub>4</sub>Si<sub>1</sub>(cr,l)

0 to 393.65 K crystal  
above 393.65 K liquid

Refer to the individual tables for details.

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa	
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [G <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	Δ <sub>f</sub> H <sup>o</sup>
	J·K <sup>-1</sup> ·mol <sup>-1</sup>	J·K <sup>-1</sup> ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>	kJ·mol <sup>-1</sup>
0				
100				
200				
298.15	108.035	258.153	0.	-189.535
300	108.198	258.822	0.200	-191.637
393.650	116.388	289.279	10.716	-189.574
393.650	163.744	339.234	30.381	-191.650
400	164.004	341.856	31.422	-191.230
500	168.134	378.897	48.029	-203.750
600	172.264	409.916	65.049	-285.814
700	176.393	436.781	82.481	-180.287
				-191.230
				-203.750
				-278.678
				-191.230
				-180.287
				-159.847
				-271.228
				-140.627
				33.574
				33.369

PREVIOUS:

CURRENT December 1977

Tetraiodosilane (SiI<sub>4</sub>)

I<sub>4</sub>Si<sub>1</sub>(cr,l)

I<sub>4</sub>Si(g)

Tetraiodosilane (SiI<sub>4</sub>)

M<sub>r</sub> = 535.7035

IDEAL GAS

Tetraiodosilane (SiI<sub>4</sub>)

S°(298.15 K) = [416.449 ± 0.21] J·K<sup>-1</sup>·mol<sup>-1</sup> ΔH°(0 K) = -105.04 ± 16.7 kJ mol<sup>-1</sup> ΔH°(298.15 K) = -110.46 ± 16.7 kJ mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies	
v, cm <sup>-1</sup>	v, cm <sup>-1</sup>
165.9(1)	404(3)
57.4(2)	88.8(3)

Ground State Quantum Weight: [1]  
 Point Group: T<sub>d</sub>  
 Bond Distance: Si-I = 2.43 ± 0.02 Å  
 Bond Angle: I-Si-I = 109° 28'  
 Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [3.653782 × 10<sup>-110</sup>] g<sup>3</sup>·cm<sup>6</sup>

Enthalpy of Formation

The sublimation, vaporization, and decomposition studies on SiI<sub>4</sub> are summarized in the following table. The vapor pressure data from the sublimation and vaporization studies are corrected for vapor non-ideality by means of the equation ΔG°/T = -R ln p - Bp/T. The Berthelot equation of state and critical constants T<sub>c</sub> = 850 K and P<sub>c</sub> = 42.1 atm as suggested by Lapidus *et al.*<sup>1</sup> are used to calculate B.

Source	Reaction	ΔH°(298.15 K), kcal·mol <sup>-1</sup>		Drift
		2nd law	3rd law	
2	A	343-396	16.23 ± 0.32	18.82 ± 0.28
3	A	eqn (flow)	18.75	19.08
3	A	eqn (static)	370-395	18.33
3	B	eqn (static)	398-425	15.68
4	B	10	399-572	15.50 ± 0.06
5	B	eqn	393-573	14.82
6	C	6	1313-1513	59.09 ± 1.14
7	C	eqn	1300-1470	59.84

Reactions: A) SiI<sub>4</sub>(cr) = SiI<sub>4</sub>(g) B) SiI<sub>4</sub>(l) = SiI<sub>4</sub>(g) C) SiI<sub>4</sub>(g) = Si(cr) + 2I<sub>2</sub>(g)

The 3rd law results of the sublimation and vaporization studies (reactions A and B) perhaps imply a better agreement among the studies than actually exists. For example, the vaporization studies of Andersen and Belz<sup>2</sup> and Uchimura *et al.*<sup>3</sup> agree very well near T<sub>sub</sub> but diverge by up to 33% as T decreases to T<sub>sub</sub>. The vapor pressure results of Bartsch and Wolf<sup>4</sup> cover a very small temperature range and lie 10-15% lower than those of Andersen and Belz<sup>2</sup> and Krichevskii *et al.*<sup>5</sup> In addition, the decomposition studies (reaction C) suggest a ΔH°(g, 298.15 K) value 3.6 kcal·mol<sup>-1</sup> more negative than the vapor pressure studies.

We adopt ΔH°(g, 298.15 K) = -26.4 kcal·mol<sup>-1</sup> based primarily on Andersen and Belz<sup>2</sup> and Krichevskii *et al.*<sup>5</sup> Andersen and Belz<sup>2</sup> are also given primary weight in our selection of S°(cr, 298.15 K). We assign an uncertainty of ±4 kcal mol<sup>-1</sup> to include the possibility that the decomposition studies<sup>3,7</sup> may be correct.

Heat Capacity and Entropy

The spectral vibrational frequencies are from the work of Clark and Rippon,<sup>8</sup> who recorded the Raman spectra in the vapor phase (210°C). The spectral data were interpreted in terms of a tetrahedral structure. This structure is consistent with the electron diffraction data of Liston and Sutton<sup>9</sup> which suggested a tetrahedral structure with a Si-I bond distance of 2.43 ± 0.02 Å. We adopt this bond distance. The principal moments of inertia are: I<sub>A</sub> = I<sub>B</sub> = I<sub>C</sub> = 331.8289 × 10<sup>-39</sup> g·cm<sup>2</sup>. Shimanouchi, in a recent compilation of molecular vibrational frequencies,<sup>10</sup> suggested somewhat different values (168, 63, 405, 94 cm<sup>-1</sup>), based on earlier infrared and Raman studies by Delwaille<sup>11</sup> and Delwaille and Francois.<sup>12</sup> Much literature has been published on the inter-relationships between force constants and vibrational frequencies. Since the majority of this work was published prior to the Clark and Rippon study,<sup>8</sup> it will not be further discussed or referenced. The same situation exists for temperature dependent thermochemical tabulations for SiI<sub>4</sub>(g).

References

1. I. Lapidus, L. A. Nisel'son and A. L. Seifer in "Thermophysical Properties of Gases and Liquids," Vol. I, V. A. Rabinovich, Ed., Israel Program for Scientific Translations, Jerusalem, pp. 102-135, (1970).
2. R. Krichevskii, G. F. Ivanovskii, and E. K. Saifonov, Zh. Fiz. Khim. 39, 2594 (1965).

Continued on page 1463

T/K	C <sub>p</sub> <sup>o</sup>	S° - [C <sub>p</sub> <sup>o</sup> - R ln(T)]/T	H <sub>f</sub> ° - H <sub>f</sub> <sup>o</sup> (T)	ΔH <sub>f</sub> <sup>o</sup>	Standard State Pressure = P° = 0.1 MPa	log K <sub>f</sub>
0	0	INFINITE	INFINITE	-105.043	-105.043	INFINITE
100	78.597	317.592	18.328	-105.538	-105.538	65.145
200	94.049	377.499	-425.478	-107.849	-107.849	63.432
250	98.051	398.948	418.092	-109.144	-109.144	61.692
298.15	100.574	416.449	416.449	-110.458	-110.458	27.988
300	100.653	417.071	0.186	-110.510	-110.510	27.869
350	102.399	432.726	417.683	-112.090	-112.090	25.102
400	103.613	446.484	420.441	-115.677	-115.677	22.854
450	104.483	458.741	424.028	-149.564	-149.564	20.712
500	105.129	469.784	428.060	-233.903	-233.903	18.159
600	105.996	489.035	436.665	-314.422	-314.422	14.092
700	106.534	495.418	445.346	-323.582	-323.582	11.965
800	106.889	519.668	453.765	-323.723	-323.723	9.028
900	107.136	532.273	461.801	-321.417	-321.417	7.347
1000	107.314	543.570	469.423	-320.909	-320.909	6.006
1100	107.447	553.805	476.636	-320.457	-320.457	4.910
1200	107.548	563.159	483.462	-320.071	-320.071	3.959
1300	107.627	571.749	489.265	-229.765	-229.765	3.229
1400	107.680	579.745	495.062	-171.011	-171.011	2.570
1500	107.741	587.180	501.892	-129.462	-129.462	1.959
1600	107.782	594.135	507.442	-138.708	-138.708	1.500
1700	107.817	600.670	512.736	-149.488	-149.488	1.045
1800	107.846	606.834	517.794	-160.272	-160.272	0.567
1900	107.871	612.665	522.635	-171.058	-171.058	0.139
2000	107.892	618.199	527.276	-181.846	-181.846	-0.246
2100	107.910	623.464	531.732	-192.636	-192.636	-0.596
2200	107.926	628.484	536.017	-203.428	-203.428	-0.914
2300	107.940	633.282	540.142	-214.219	-214.219	-1.205
2400	107.951	637.876	544.119	-225.015	-225.015	-1.473
2500	107.962	642.283	547.958	-235.811	-235.811	-1.720
2600	107.971	646.517	551.668	-246.608	-246.608	-1.949
2700	107.980	650.592	555.257	-257.404	-257.404	-2.162
2800	107.987	654.520	558.732	-268.204	-268.204	-2.360
2900	107.994	658.309	562.101	-279.003	-279.003	-2.546
3000	108.000	661.970	565.369	-289.556	-289.556	-2.719
3100	108.006	665.512	568.543	-299.222	-299.222	-2.882
3200	108.011	668.941	571.627	-311.404	-311.404	-3.035
3300	108.015	672.265	574.627	-323.205	-323.205	-3.179
3400	108.019	675.489	577.546	-333.007	-333.007	-3.315
3500	108.023	678.621	580.389	-343.809	-343.809	-3.443
3600	108.027	681.664	583.161	-354.611	-354.611	-3.571
3700	108.030	684.624	585.863	-365.414	-365.414	-3.702
3800	108.033	687.505	588.500	-376.217	-376.217	-3.838
3900	108.036	690.311	591.075	-387.021	-387.021	-3.979
4000	108.038	693.046	593.590	-397.825	-397.825	-4.124
4100	108.041	695.714	596.048	-408.628	-408.628	-4.272
4200	108.043	698.317	598.452	-419.433	-419.433	-4.421
4300	108.045	700.860	600.805	-430.237	-430.237	-4.571
4400	108.047	703.344	603.107	-441.042	-441.042	-4.721
4500	108.049	705.772	605.361	-451.846	-451.846	-4.871
4600	108.050	708.147	607.570	-462.651	-462.651	-5.021
4700	108.052	710.470	609.735	-473.456	-473.456	-5.171
4800	108.053	712.745	611.857	-484.261	-484.261	-5.321
4900	108.055	714.973	613.939	-495.067	-495.067	-5.471
5000	108.056	717.156	615.982	-505.872	-505.872	-5.621
5100	108.057	719.296	617.987	-516.678	-516.678	-5.771
5200	108.058	721.394	619.955	-527.483	-527.483	-5.921
5300	108.059	723.453	621.888	-538.288	-538.288	-6.071
5400	108.060	725.478	623.788	-549.093	-549.093	-6.221
5500	108.061	727.455	625.655	-559.900	-559.900	-6.371
5600	108.062	729.402	627.490	-570.708	-570.708	-6.521
5700	108.063	731.315	629.295	-581.514	-581.514	-6.671
5800	108.064	733.195	631.070	-592.321	-592.321	-6.821
5900	108.065	735.042	632.817	-603.127	-603.127	-6.971
6000	108.066	736.858	634.536	-613.934	-613.934	-7.121

PREVIOUS December 1977 (1 atm) CURRENT December 1977 (1 bar)

Tetraiodosilane (SiI<sub>4</sub>)

I<sub>4</sub>Si(g)

**Titanium Iodide (TiI<sub>4</sub>)**

**Titanium Iodide (TiI<sub>4</sub>)**

*M<sub>r</sub>* = 555.4980

**CRYSTAL**

**Titanium Iodide (TiI<sub>4</sub>)**

*S*<sup>o</sup>(298.15 K) = 246.150 ± 6.7 J·K<sup>-1</sup>·mol<sup>-1</sup>  
*T<sub>m</sub>* = 379 K  
*T<sub>liq</sub>* = 428 K  
 $\Delta_f H^\circ(0 \text{ K}) = -373.64 \pm 8.4 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15 \text{ K}) = -375.72 \pm 8.4 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{cr}} H^\circ = 9.16 \pm 0.63 \text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_{\text{liq}} H^\circ = 19.832 \pm 0.63 \text{ kJ}\cdot\text{mol}^{-1}$

**Enthalpy of Formation**

The enthalpy of formation of TiI<sub>4</sub>(cr) was measured by Johnson *et al.*<sup>1</sup> based on the enthalpies of hydrolysis of TiBr<sub>4</sub>(cr) and TiI<sub>4</sub>(cr) in sulfuric acid. These data result in an enthalpy of reaction of -57.88 kcal·mol<sup>-1</sup> for the process TiI<sub>4</sub>(cr) + 2Br<sub>2</sub>(l) = TiBr<sub>4</sub>(cr) + 2I<sub>2</sub>(cr), when recalculated with revised values of  $\Delta_f H^\circ(298.15 \text{ K})$  for HBr(aq) and HI(aq).<sup>2</sup> Combination of  $\Delta_f H^\circ(298.15 \text{ K})$  with auxiliary JANAF data gives the adopted value of  $\Delta_f H^\circ(298.15 \text{ K})$ .

**Heat Capacity and Entropy**

King *et al.*<sup>1</sup> reported the heat capacity and enthalpy of TiI<sub>4</sub>(cr) over the temperature range 51 to 428 K. The value of *S*<sup>o</sup>(298.15 K) is calculated from these data based on *S*<sup>o</sup>(51 K) = 14.62 cal·K<sup>-1</sup>·mol<sup>-1</sup>. The value of *H*<sup>o</sup>(51 K) - *H*<sup>o</sup>(0 K) is calculated to be 0.356 kcal·mol<sup>-1</sup> from a Debye Einstein extrapolation of the measured heat capacities.

**Transition Data**

A first order transition was observed by King *et al.*<sup>1</sup> at 379 K. They reported the measured value of 2.37 kcal·mol<sup>-1</sup>, noting that this value had an uncertainty of 0.15 kcal·mol<sup>-1</sup> due to hysteresis in the transition.

**Fusion Data**

The melting temperature and enthalpy of fusion were reported by King *et al.*<sup>2</sup> The large uncertainty of  $\Delta_{\text{liq}} H^\circ$  is due to the uncertainty and close proximity of the transition at 379 K.

**References**

- W. H. Johnson, A. A. Gilliland, and E. J. Prosen, *J. Res. Nat. Bur. Stand.* **63A**, 161 (1959).
- U. S. Nat. Bur. Stand. *Techn. Note* **270-3**, (1968).
- E. G. King, W. W. Weller, A. U. Christensen and K. K. Kelley, *U. S. Bur. Mines RI* **5799**, (1961).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p <sup>o</sup> = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - (G <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> ))/T	H <sup>o</sup> - H <sup>o</sup> (T <sub>r</sub> )	Δ <sub>f</sub> H <sup>o</sup>	
0	0.	0.	INFINITE	-373.638	INFINITE
100	100.671	120.059	352.958	-374.448	195.059
200	119.349	197.192	257.466	-374.995	97.210
298.15	125.629	246.150	246.150	-370.687	64.943
300	125.947	246.928	246.153	-370.655	64.537
379.000	139.608	277.904	249.613	-370.655	64.537
379.000	148.114	304.068	249.613	-370.655	64.537
400	148.114	312.056	252.683	-370.655	64.537
428.000	148.114	322.077	256.899	-370.655	64.537
500	148.114	345.106	267.986	-370.655	64.537
600	148.114	372.111	283.158	-370.655	64.537
700	148.114	394.942	297.538	-370.655	64.537
800	148.114	414.720	310.977	-370.655	64.537
900	148.114	432.166	323.492	-370.655	64.537
1000	148.114	447.771	335.154	-370.655	64.537
1100	148.114	461.888	346.044	-370.655	64.537
1200	148.114	474.775	356.242	-370.655	64.537
1300	148.114	486.631	365.822	-370.655	64.537
1400	148.114	497.607	374.848	-370.655	64.537
1500	148.114	507.826	383.376	-370.655	64.537

TRANSITION  
 I < -> II  
 -368.316  
 -352.801  
 -337.296  
 -320.534  
 -278.397  
 -254.797  
 -231.662  
 -208.926  
 -186.412  
 -163.998  
 -141.896  
 -120.072

PREVIOUS: June 1964

CURRENT: December 1968

**Titanium Iodide (TiI<sub>4</sub>)**

**TiI<sub>4</sub>(cr)**

Titanium Iodide (TiI<sub>4</sub>)

## LIQUID

M<sub>r</sub> = 555.4980Titanium Iodide (TiI<sub>4</sub>)I<sub>4</sub>Ti<sub>1</sub>(l)

$$S^{\circ}(298.15 \text{ K}) = [311.841] \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$$

$$T_{\text{fus}} = 428 \text{ K}$$

## Enthalpy of Formation

$\Delta_f H^{\circ}(\text{TiI}_4, l, 298.15 \text{ K})$  is calculated from  $\Delta_f H^{\circ}(\text{TiI}_4, cr, 298.15 \text{ K})$  by adding the enthalpy of fusion,  $\Delta_{\text{fus}} H^{\circ}$ , and the difference in enthalpy,  $H^{\circ}(428 \text{ K}) - H^{\circ}(298.15 \text{ K})$ , between the crystal and liquid.

## Heat Capacity and Entropy

King *et al.* reported the enthalpy of TiI<sub>4</sub>(l) above the melting temperature. The heat capacity derived from these data is constant.  $S^{\circ}(\text{TiI}_4, l, 298.15 \text{ K})$  is calculated in a manner analogous to that used for the enthalpy of formation.

## Fusion Data

The melting temperature and enthalpy of fusion were reported by King *et al.*<sup>1</sup>

## Vaporization Data

The boiling temperature,  $T_{\text{vap}}$ , is taken as the temperature at which the fugacity is 1 bar for the reaction  $\text{TiI}_4(l) = \text{TiI}_4(g)$ . The enthalpy of vaporization is calculated as the difference between  $\Delta_f H^{\circ}$  of the liquid and gas at the boiling temperature. The vapor pressure data are discussed in the table for TiI<sub>4</sub>(g).

## Reference

<sup>1</sup>E. G. King, W. W. Weller, A. U. Christensen, and K. K. Kelley, U. S. Bur. Mines RI 5799, 20 pp. (1961).

T/K	C <sub>p</sub> <sup>o</sup>	S <sup>o</sup> - [C <sub>p</sub> <sup>o</sup> - H <sup>o</sup> (T)]/T	H <sup>o</sup> - H <sup>o</sup> (T)	Δ <sub>f</sub> H <sup>o</sup>	Δ <sub>f</sub> G <sup>o</sup>	log K <sub>r</sub>
0						
100						
200						
298.15	156.482	311.841	0.	-348.314	-362.863	63.572
300	156.482	311.844	0.289	-348.273	-362.954	63.196
400	156.482	317.826	15.938	-378.515	-367.027	47.929
428.000	156.482	320.939	20.319	---	LIQUID	---
500	156.482	329.573	31.586	-462.000	-356.185	37.210
600	156.482	349.551	47.234	-456.685	-335.523	29.210
700	156.482	375.566	62.882	-451.460	-315.744	23.561
800	156.482	405.291	78.530	-446.295	-296.709	19.373
900	156.482	444.722	94.178	-441.219	-278.316	16.153
1000	156.482	501.209	109.827	-436.295	-260.482	13.606
1100	156.482	516.123	125.475	-431.593	-243.130	11.545
1200	156.482	529.739	141.123	-431.105	-226.076	9.841
1300	156.482	542.264	156.771	-426.149	-209.193	8.405
1400	156.482	553.861	172.419	-421.333	-192.685	7.189
1500	156.482	564.657	188.067	-416.690	-176.516	6.147

Enthalpy Reference Temperature = T<sub>r</sub> = 298.15 K

PREVIOUS June 1964

CURRENT December 1968

Titanium Iodide (TiI<sub>4</sub>)I<sub>4</sub>Ti<sub>1</sub>(l)





Titanium Iodide (TiI<sub>4</sub>)

IDEAL GAS

M<sub>r</sub> = 555.4980

I<sub>4</sub>Ti<sub>1</sub>(g)

S°(298.15 K) = 433.072 ± 8.4 J·K<sup>-1</sup>·mol<sup>-1</sup>

ΔH<sup>o</sup>(298.15 K) = -277.27 ± 8.4 kJ·mol<sup>-1</sup>

ΔH<sup>o</sup>(0 K) = -271.86 ± 8.4 kJ·mol<sup>-1</sup>

Vibrational Frequencies and Degeneracies

v, cm <sup>-1</sup>	v, cm <sup>-1</sup>
[175](1)	[260](3)
[55](2)	[69](3)

Ground State Quantum Weight: 1

Point Group: T<sub>d</sub>

Bond Distance: Ti-I = [2.5] Å

Bond Angle: I-Ti-I = [109°28']

Product of the Moments of Inertia: I<sub>A</sub>I<sub>B</sub>I<sub>C</sub> = [4.332573 × 10<sup>-109</sup>] g<sup>3</sup>·cm<sup>6</sup>

σ = 12

Enthalpy of Formation

The enthalpy of formation of TiI<sub>4</sub>(g) is calculated from that of TiI<sub>4</sub>(l) and the enthalpy of vaporization of the liquid. Blocher and Campbell<sup>1</sup> reported vapor pressure data for TiI<sub>4</sub>(l) over the temperature range 473 to 655 K. 2nd and 3rd law analyses of these data give values for Δ<sub>vap</sub>H°(298.15 K) of 17.2 ± 0.1 and 16.98 kcal·mol<sup>-1</sup>, respectively, the 3rd law drift being -0.4 ± 0.2 cal·K<sup>-1</sup>·mol<sup>-1</sup>. The adopted value of ΔH°(298.15 K) is based on the 3rd law enthalpy of vaporization.

Heat Capacity and Entropy

The interatomic distances are estimated from those of TiBr<sub>4</sub>(cr), TiBr<sub>4</sub>(g) and TiI<sub>4</sub>(cr).<sup>2</sup> The tetrahedral model is assumed by analogy with TiCl<sub>4</sub>(g) and TiBr<sub>4</sub>(g). The principal moments of inertia are: I<sub>A</sub> = I<sub>B</sub> = I<sub>C</sub> = 351.2222 × 10<sup>-39</sup> g·cm<sup>2</sup>.

The vibrational frequencies of TiI<sub>4</sub>(g) have been estimated by Ushanova *et al.*<sup>3</sup> The given estimates are based on their predictions and valence force field calculations.

References

- 1 J. M. Blocher, Jr. and I. E. Campbell, *J. Amer. Chem. Soc.* **69**, 2100 (1947).
- 2 O. Hassel and H. Kringstand, *Z. Phys. Chem.* **1315**, 274 (1932).
- 3 N. I. Ushanova, I. N. Godnev and I. V. Orlova, *Opt. Spektrosk.* **5**, 567 (1958).

Titanium Iodide (TiI<sub>4</sub>)

T/K	C <sub>p</sub> <sup>o</sup>	Enthalpy Reference Temperature = T, = 298.15 K		Standard State Pressure = P° = 0.1 MPa		log K <sub>f</sub>
		S° - (G° - H°(T))/T	H° - H°(T)	ΔG°	ΔG°	
0	0	INFINITE	0	INFINITE	-271.860	INFINITE
100	85.757	372.171	522.445	-19.527	-272.236	152.488
200	100.193	392.170	442.507	-10.068	-274.558	81.163
250	102.779	414.832	434.781	-4.987	-275.896	66.790
298.15	104.254	433.072	433.072	0	-277.274	57.459
300	104.298	433.717	433.074	0.193	-277.329	57.159
350	105.256	449.872	434.347	5.433	-278.999	50.242
400	105.895	463.971	437.188	10.713	-281.699	44.878
450	106.342	476.471	440.871	16.070	-284.816	40.313
500	106.666	487.693	445.002	21.345	-287.292	35.818
600	107.093	507.181	453.789	32.035	-290.844	28.836
700	107.354	523.354	462.627	42.759	-294.543	23.832
800	107.524	538.058	471.179	53.503	-298.109	20.117
900	107.641	550.730	479.328	64.262	-301.600	17.214
1000	107.726	562.075	487.045	75.030	-305.051	14.892
1100	107.788	572.346	494.340	85.806	-308.421	12.992
1200	107.836	581.727	501.237	96.587	-311.657	11.403
1300	107.873	590.360	507.765	107.373	-314.782	10.048
1400	107.902	598.355	513.954	118.162	-317.814	8.887
1500	107.926	605.800	519.832	128.953	-320.764	7.881
1600	107.945	612.766	525.425	139.747	-323.636	6.999
1700	107.962	619.311	530.757	150.542	-326.433	6.221
1800	107.975	625.482	535.850	161.339	-329.160	5.527
1900	107.987	631.320	540.722	172.137	-331.827	4.905
2000	107.996	636.860	545.392	182.936	-334.434	4.332
2100	108.005	642.129	549.874	193.736	-336.981	3.803
2200	108.012	647.154	554.182	204.537	-339.478	3.319
2300	108.019	651.955	558.330	215.339	-341.925	2.874
2400	108.024	656.532	562.327	226.141	-344.321	2.464
2500	108.029	660.982	566.185	236.943	-346.668	2.084
2600	108.034	665.199	569.912	247.747	-348.964	1.731
2700	108.037	669.277	573.517	258.550	-351.211	1.402
2800	108.041	673.206	577.008	269.354	-353.418	1.094
2900	108.044	676.997	580.391	280.158	-355.585	0.806
3000	108.047	680.660	583.672	290.963	-357.721	0.535
3100	108.049	684.203	586.859	301.768	-359.828	0.280
3200	108.052	687.633	589.954	312.573	-361.905	0.039
3300	108.054	690.958	592.965	323.378	-363.952	-0.188
3400	108.056	694.184	595.895	334.184	-365.970	-0.403
3500	108.058	697.316	598.748	344.989	-367.960	-0.608
3600	108.059	700.361	601.529	355.795	-369.922	-0.801
3700	108.061	703.321	604.240	366.601	-371.856	-1.095
3800	108.062	706.203	606.885	377.407	-373.763	-1.423
3900	108.063	709.019	609.468	388.213	-375.643	-1.733
4000	108.063	711.746	611.991	399.020	-377.500	-2.029
4100	108.066	714.414	614.457	409.826	-379.333	-2.310
4200	108.067	717.019	616.868	420.633	-381.143	-2.578
4300	108.068	719.561	619.227	431.440	-382.929	-2.834
4400	108.069	722.046	621.535	442.247	-384.692	-3.078
4500	108.069	724.475	623.796	453.053	-386.432	-3.311
4600	108.070	726.850	626.011	463.860	-388.149	-3.535
4700	108.071	729.174	628.181	474.667	-389.843	-3.749
4800	108.072	731.449	630.309	485.475	-391.514	-3.954
4900	108.072	733.678	632.396	496.282	-393.162	-4.151
5000	108.073	735.861	634.443	507.089	-394.787	-4.340
5100	108.073	738.001	636.453	517.896	-396.389	-4.522
5200	108.074	740.100	638.426	528.704	-397.968	-4.697
5300	108.074	742.158	640.364	539.511	-399.525	-4.865
5400	108.075	744.178	642.268	550.319	-401.060	-5.027
5500	108.075	746.162	644.139	561.126	-402.573	-5.183
5600	108.076	748.109	645.978	571.934	-404.064	-5.333
5700	108.076	750.022	647.786	582.741	-405.533	-5.478
5800	108.077	751.901	649.565	593.549	-406.981	-5.618
5900	108.077	753.749	651.316	604.356	-408.408	-5.754
6000	108.077	755.565	653.038	615.164	-409.814	-5.884

PREVIOUS: December, 1968 (1 atm)

CURRENT: December, 1968 (1 bar)

Titanium Iodide (TiI<sub>4</sub>)

I<sub>4</sub>Ti<sub>1</sub>(g)

Zirconium Iodide (ZrI<sub>4</sub>)

## CRYSTAL

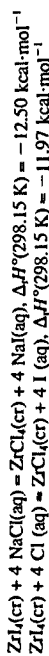
M<sub>r</sub> = 598.8380 Zirconium Iodide (ZrI<sub>4</sub>)I<sub>4</sub>Zr<sub>1</sub>(cr)

S°(298.15 K) = [260.270 ± 4.2] J·K<sup>-1</sup>·mol<sup>-1</sup>  
 T<sub>fus</sub> = 772 ± 2 K  
 T<sub>sub</sub> = 705.6 K

ΔH<sup>o</sup>(0 K) = [-487.24 ± 8.4] kJ·mol<sup>-1</sup>  
 ΔH<sup>o</sup>(298.15 K) = -488.69 ± 6.3 kJ·mol<sup>-1</sup>  
 Δ<sub>sub</sub>H<sup>o</sup> = Unknown  
 Δ<sub>sub</sub>H<sup>o</sup>(298.15 K) = 126.357 ± 2.1 kJ·mol<sup>-1</sup>

## Enthalpy of Formation

<sup>1</sup>Turnbull<sup>1</sup> measured the enthalpies of reaction for the dissolution of the zirconium tetrahalides in caustic and in water. The reported enthalpies of reaction and the corresponding reactions may be combined to yield the following:



Using auxiliary data,<sup>2,4</sup> we calculate Δ<sub>f</sub>H<sup>o</sup>(298.15 K) = -116.52 and -117.05 kcal·mol<sup>-1</sup> for ZrI<sub>4</sub>(cr) from these two reactions. We adopt a mean of these two values, Δ<sub>f</sub>H<sup>o</sup>(298.15 K) = -116.8 kcal·mol<sup>-1</sup>, and assign an uncertainty of ±1.5 kcal·mol<sup>-1</sup>. The value suggested by NBS<sup>3</sup> is 1.7 kcal·mol<sup>-1</sup>, more positive.

Baev and Shelton<sup>5</sup> reference an enthalpy of formation value for ZrI<sub>4</sub>(cr). The reported Δ<sub>f</sub>H<sup>o</sup>(298.15 K) = 105.9 kcal·mol<sup>-1</sup>, as supposedly extracted from Karapet'yants and Karapet'yants.<sup>6</sup> We tentatively discard this value due to the large number of inconsistencies in the reported tabular results of Baev and Shelton.<sup>5</sup>

## Heat Capacity and Entropy

There is no heat capacity and enthalpy data reported in the literature for ZrI<sub>4</sub>(cr). The adopted heat capacity values are estimated such they parallel those adopted for ZrCl<sub>4</sub>(cr) and ZrBr<sub>4</sub>(cr)<sup>7</sup> and are consistent with the sublimation data.

The crystal data compilation of Donnay and Ondik<sup>8</sup> does not list the crystal structure of ZrI<sub>4</sub>(cr) but does tabulate both ZrCl<sub>4</sub> and ZrBr<sub>4</sub> as cubic structures. The literature data related to the crystal structure of ZrI<sub>4</sub> is not definitive. Assuming ZrI<sub>4</sub>(cr) also has a cubic structure, the adopted heat capacity values are estimated so as to parallel those for ZrCl<sub>4</sub> and ZrBr<sub>4</sub>. The values below 300 K are calculated in the same manner as for ZrBr<sub>4</sub>(cr).<sup>7</sup> The high temperature heat capacities are obtained graphically.

## Fusion Data

The melting point was observed by Rahlfs and Fischer<sup>9</sup> to be 772 ± 2 K and by Nisel'son<sup>10</sup> to be 773 K.

## Sublimation Data

The sublimation data are treated in the ZrI<sub>4</sub>(g) table.<sup>2</sup> The sublimation temperature, T<sub>sub</sub>, is calculated from the Gibbs energy crossover between the crystal and gas. Since T<sub>sub</sub> is less than T<sub>fus</sub>, the liquid phase is thermodynamically unstable at one atmosphere pressure.

## References

- <sup>1</sup>A. G. Turnbull, *J. Phys. Chem.*, **65**, 1652 (1961).
- <sup>2</sup>JANAF Thermochemical Tables: ZrCl<sub>4</sub>(cr), ZrBr<sub>4</sub>(cr) and ZrI<sub>4</sub>(g), 6-30-75.
- <sup>3</sup>U. S. Nat. Bur. Stand. Tech. Note 270-5, (1971).
- <sup>4</sup>ICSD CODATA Task Group, *J. Chem. Thermodyn.*, **4**, 331 (1972).
- <sup>5</sup>A. K. Baev and R. A. J. Shelton, *Russ. J. Phys. Chem.*, **47**, 1340 (1973).
- <sup>6</sup>M. K. Karapet'yants and M. L. Karapet'yants, "Osnovnye Termokhimitseskie Konstanty Neorganicheskikh i Organicheskikh Veshchestv," Izd. Khimiya, Moscow, 1968 (as referenced by Baev and Shelton).<sup>3</sup>
- <sup>7</sup>F. R. Sale and R. A. J. Shelton, *J. Less Common Metals*, **9**, 54 (1965).
- <sup>8</sup>J. D. H. Donnay and H. M. Ondik, "Crystal Data, Determinative Tables," 3rd edition, Vol. 2, U. S. Nat. Bur. Stand. and Joint Committee on Powder Diffraction Standards, (1973).
- <sup>9</sup>O. Rahlfs and W. Fischer, *Z. anorg. allg. Chem.*, **211**, 349 (1933).
- <sup>10</sup>L. A. Nisel'son, *Russ. J. Inorg. Chem.*, **7**, 354 (1962).

T/K	Enthalpy Reference Temperature = T <sub>r</sub> = 298.15 K		Standard State Pressure = p° = 0.1 MPa		log K <sub>r</sub>
	C <sub>p</sub> <sup>o</sup>	S° - [G° - H°(T <sub>r</sub> )]/T	H° - H°(T <sub>r</sub> )	Δ <sub>f</sub> G°	
0	0	0	INFINITE	-487.236	INFINITE
100	104.207	131.545	369.071	-487.537	254.428
200	121.579	210.426	271.784	-488.114	177.036
298.15	127.800	260.270	260.270	-488.691	85.048
300	127.880	261.061	260.272	-488.703	84.520
400	131.001	298.303	265.379	-485.426	63.087
500	133.009	327.759	274.971	-483.104	48.603
600	134.598	352.154	285.860	-480.216	38.053
700	135.938	373.005	296.836	-476.990	30.538
800	137.152	391.236	307.537	-472.743	24.967
900	138.245	407.460	317.755	-467.496	20.641
1000	139.278	422.101	327.469	-461.258	17.200

PREVIOUS: June 1964

CURRENT: June 1975

Zirconium Iodide (ZrI<sub>4</sub>)I<sub>4</sub>Zr<sub>1</sub>(cr)

$I_4Zr_1(g)$

Zirconium Iodide ( $ZrI_4$ )

$M_r = 598.8380$

IDEAL GAS

Zirconium Iodide ( $ZrI_4$ )

$\Delta_f H^\circ(0\text{ K}) = -356.75 \pm 8.4\text{ kJ}\cdot\text{mol}^{-1}$   
 $\Delta_f H^\circ(298.15\text{ K}) = -362.33 \pm 8.4\text{ kJ}\cdot\text{mol}^{-1}$

Vibrational Frequencies and Degeneracies  
 $\nu, \text{cm}^{-1}$

- 158 (1)
- 43 (2)
- 254 (3)
- 55 (3)

Ground State Quantum Weight: [1]  $\sigma = 12$

Point Group:  $T_d$

Bond Distance:  $Zr-I = 2.660 \pm 0.005\text{ \AA}$

Bond Angle:  $I-Zr-I = 109^\circ 28'$

Product of the Moments of Inertia:  $I_A I_B I_C = 6.286307 \times 10^{-10}\text{ g}^3\cdot\text{cm}^6$

**Enthalpy of Formation**

The enthalpy of formation for  $ZrI_4(g)$  is calculated from the enthalpies of formation and sublimation at 298.15 K. The adopted value for the heat of sublimation,  $\Delta_{sub} H^\circ(298.15\text{ K}) = 30.2 \pm 0.5\text{ kcal}\cdot\text{mol}^{-1}$ , is based on the 2nd and 3rd law analyses of the sublimation data of Sale and Shelton<sup>1</sup> and Rahlfs and Fischer.<sup>2</sup> Using Knudsen effusion techniques, Sale and Shelton<sup>1</sup> studied effusion in a nickel effusion cell for three different orifice areas. The results were then extrapolated to zero orifice area (refer to last line in the following table). Other sublimation studies have been conducted by Rahlfs and Fischer,<sup>2</sup> using a liquid tin tensimeter, and by Gerlach *et al.*,<sup>3</sup> using the oscillating quartz fiber method. It should be noted that the work of Rahlfs and Fischer<sup>2</sup> covered an observed pressure range of 4.0–272 mm Hg, which is much wider than range covered by Sale and Shelton.<sup>1</sup> The adopted  $\Delta_{sub} H^\circ(298.15\text{ K})$  is based on the mean of the 3rd law results of Sale and Shelton (30.01 kcal·mol<sup>-1</sup>), and Rahlfs and Fischer (30.32 kcal·mol<sup>-1</sup>).

The effusion studies (membrane method) by Baev and Shelton<sup>4</sup> are discarded due to the large number of discrepancies in their tabulated results.

In analyzing the vapor pressures for the three sublimation studies,<sup>1,2,3</sup> corrections were made for non-ideality by means of the equation  $\Delta G^\circ/T = -R \ln p - Bp/T$ . The Bertholet equation of state and the critical constants  $T_c = 959\text{ K}$  and  $p_c = 40.7\text{ atm}$  as determined by Nisel<sup>5</sup> and Sokolova<sup>6</sup> are used to calculate B.

Source	T/K	Data Points	$\Delta_{sub} H^\circ(298.15\text{ K}), \text{kcal}\cdot\text{mol}^{-1}$	Drift	
2	558–671	15*	31.33 ± 0.24	30.32 ± 0.12	-1.62 ± 0.38
3	393–453	eqn	26.91	29.98	7.25
1	426–474A**	12*	29.84 ± 1.28	31.22 ± 0.30	3.09 ± 2.84
	432–500B**	14*	30.81 ± 0.57	30.86 ± 0.15	0.10 ± 1.24
	436–480C**	12	30.24 ± 0.76	30.51 ± 0.17	0.61 ± 1.66
	423–503	eqn	29.97	30.01	0.08

\*One point rejected due to a statistical test

\*\*Orifice area (cm<sup>2</sup> 10<sup>3</sup>) A = 0.5364 B = 0.0935

**Heat Capacity and Entropy**

The adopted vibrational frequencies are from the work of Clark *et al.*,<sup>6,7</sup> who recorded the Raman spectra of  $ZrI_4$  in the vapor phase (380–420°C). These studies indicated that  $ZrI_4$  is a tetrahedral monomer in the vapor phase. Shimanouchi, in his compilation of molecular vibrational frequencies,<sup>8</sup> also adopted the values of Clark *et al.*<sup>6,7</sup> for  $ZrI_4(g)$ . Rahlfs and Fischer,<sup>2</sup> though vapor density measurements had earlier concluded that  $ZrI_4$  was monomeric in the vapor phase.

An electron diffraction study of  $ZrI_4(g)$  at 250–270°C was conducted by Zasorin *et al.*<sup>9</sup> This study confirmed the tetrahedral structure and determined the  $Zr-I$  bond length to be  $2.660 \pm 0.005\text{ \AA}$ . We adopt this value. Other interatomic distances reported in the literature are estimates. The principal moments of inertia are:  $I_A = I_B = I_C = 397.6172 \times 10^{-39}\text{ g}\cdot\text{cm}^2$ .

Much literature has been published on the inter-relationships between force constants and vibrational frequencies. Since the majority of these are based on estimated frequencies, they will not be further discussed or referenced. The same situation is true for thermodynamic tabulations of  $ZrI_4(g)$ . One exception is that Clark *et al.*<sup>6</sup> calculated thermodynamic properties based on their experimental vibrational frequencies. Their tabulation is very similar to ours the differences in the entropy being  $0.04\text{ cal}\cdot\text{K}^{-1}\cdot\text{mol}^{-1}$  in the range 100–1000 K.

Continued on page 1463

Zirconium Iodide ( $ZrI_4$ )

$I_4Zr_1(g)$

T/K	$C_p^\circ$	$S^\circ$	$-(G^\circ - H^\circ(T))/T$	$H^\circ - H^\circ(T)$	$\Delta_f H^\circ$	$\Delta_f G^\circ$	log K <sub>r</sub>
Enthalpy Reference Temperature = $T_r = 298.15\text{ K}$		Standard State Pressure = $p^\circ = 0.1\text{ MPa}$					
J·K <sup>-1</sup> ·mol <sup>-1</sup>		J·K <sup>-1</sup> ·mol <sup>-1</sup>		KJ·mol <sup>-1</sup>		log K <sub>r</sub>	
0	0	0	INFINITE	-26.311	-356.752	-356.752	INFINITE
100	87.629	339.627	536.514	-19.689	-357.116	-357.116	197.173
200	100.873	403.465	436.038	-10.115	-359.600	-359.600	103.660
298.15	103.241	428.234	448.278	-5.006	-360.962	-360.962	84.843
300	104.589	446.563	446.563	0	-362.334	-362.334	72.642
350	104.629	447.210	446.565	0.194	-362.389	-362.389	63.250
400	105.504	463.409	447.843	5.448	-364.079	-364.079	52.618
450	106.088	470.538	450.690	10.739	-367.679	-367.679	43.246
500	106.496	480.054	454.382	16.054	-371.106	-371.106	36.070
550	106.791	501.295	458.521	21.387	-376.658	-376.658	30.491
600	107.181	520.803	467.324	32.087	-384.549	-384.549	26.532
700	107.418	537.344	476.175	42.818	-395.119	-395.119	23.496
800	107.574	551.698	484.738	53.568	-397.780	-397.780	21.572
900	107.681	564.375	492.896	64.331	-398.921	-398.921	20.456
1000	107.758	575.725	500.622	75.103	-398.081	-398.081	19.644
1100	107.814	585.982	507.974	85.882	-396.246	-396.246	17.344
1200	107.858	595.381	514.826	96.666	-393.584	-393.584	15.417
1300	107.892	604.016	521.359	107.453	-390.111	-390.111	13.782
1400	107.919	612.012	527.553	118.244	-385.823	-385.823	12.382
1500	107.940	619.459	533.434	129.037	-380.697	-380.697	11.168
1600	107.958	626.426	539.031	139.832	-374.825	-374.825	10.105
1700	107.973	632.971	544.366	150.628	-368.216	-368.216	9.167
1800	107.985	639.143	549.462	161.426	-360.900	-360.900	8.335
1900	107.996	644.982	554.337	172.225	-353.002	-353.002	7.583
2000	108.003	650.521	559.009	183.025	-344.607	-344.607	6.911
2100	108.012	655.791	563.493	193.826	-335.821	-335.821	6.299
2200	108.019	660.816	567.803	204.628	-326.748	-326.748	5.724
2300	108.025	665.618	571.953	215.430	-317.387	-317.387	5.191
2400	108.030	670.215	575.952	226.233	-307.842	-307.842	4.700
2500	108.034	674.625	579.811	237.036	-298.124	-298.124	4.247
2600	108.038	678.863	583.540	247.839	-288.335	-288.335	3.826
2700	108.042	682.940	587.146	258.643	-278.470	-278.470	3.435
2800	108.045	686.869	590.638	269.448	-268.532	-268.532	3.070
2900	108.048	690.661	594.022	280.252	-258.521	-258.521	2.728
3000	108.050	694.324	597.305	291.055	-248.436	-248.436	2.408
3100	108.053	697.867	600.492	301.863	-238.271	-238.271	2.107
3200	108.055	701.298	603.589	312.668	-228.034	-228.034	1.824
3300	108.057	704.623	606.600	323.474	-217.725	-217.725	1.557
3400	108.059	707.848	609.531	334.279	-207.346	-207.346	1.304
3500	108.060	710.981	612.385	345.085	-196.893	-196.893	1.066
3600	108.062	714.025	615.166	355.891	-186.366	-186.366	0.839
3700	108.063	716.986	617.878	366.698	-175.771	-175.771	0.624
3800	108.064	719.868	620.525	377.504	-165.118	-165.118	0.420
3900	108.066	722.675	623.108	388.310	-154.407	-154.407	0.226
4000	108.067	725.411	625.631	399.117	-143.640	-143.640	0.041
4100	108.068	728.079	628.098	409.924	-132.820	-132.820	-0.136
4200	108.069	730.683	630.509	420.731	-121.950	-121.950	-0.304
4300	108.069	733.226	632.869	431.537	-111.034	-111.034	-0.465
4400	108.070	735.711	635.178	442.344	-100.076	-100.076	-0.619
4500	108.071	738.139	637.439	453.152	-89.080	-89.080	-0.766
4600	108.072	740.515	639.654	463.959	-78.044	-78.044	-0.907
4700	108.072	742.839	641.825	474.766	-66.968	-66.968	-1.042
4800	108.073	745.114	643.953	485.573	-55.852	-55.852	-1.178
4900	108.074	747.343	646.040	496.380	-44.697	-44.697	-1.313
5000	108.074	749.526	648.088	507.188	-33.505	-33.505	-1.447
5100	108.075	751.666	650.098	517.995	-22.270	-22.270	-1.581
5200	108.075	753.765	652.072	528.801	-11.000	-11.000	-1.716
5300	108.076	755.823	654.010	539.610	0.300	0.300	-1.851
5400	108.076	757.844	655.914	550.418	11.500	11.500	-1.986
5500	108.076	759.827	657.786	561.225	22.700	22.700	-2.121
5600	108.077	761.774	659.625	572.033	33.900	33.900	-2.256
5700	108.077	763.687	661.434	582.841	45.100	45.100	-2.391
5800	108.077	765.567	663.213	593.649	56.300	56.300	-2.526
5900	108.078	767.414	664.964	604.456	67.500	67.500	-2.661
6000	108.078	769.231	666.687	615.264	78.700	78.700	-2.796

PREVIOUS: June 1975 (1 atm)

CURRENT: June 1975 (1 bar)

## Iodine

## Continued from page 1404

- <sup>6</sup>D. St. A. G. Radlein, J. C. Whitehead and R. Grice, *Nature* **253**, 37 (1975).  
<sup>7</sup>R. J. Buss, S. J. Sibener and Y. T. Lee, *J. Phys. Chem.* **87**(24), 4840 (1983).  
<sup>8</sup>B. Ruscic and J. Berkowitz, *J. Chem. Phys.* **101**(9), 7795 (1994).  
<sup>9</sup>JANAF Thermochemical Tables: I(g), June 1982, I<sub>2</sub>(ref), June 1982; O(g), June 1982; O<sub>2</sub>(ref), June (1982).  
<sup>10</sup>P. S. Monks, L. J. Stief, D. C. Tardy, F. Liebman, Z. Zhang, S.-C. Kuo and R. B. Klemm, *J. Phys. Chem.*, (submitted for publication July 1995).  
<sup>11</sup>G. Herzberg, *Spectra of Diatomic Molecules*, D. Van Nostrand Co., New York, p. 107 (1950).  
<sup>12</sup>J. P. Bekooj, W. L. Meerts, and A. Dynamus, *J. Mol. Spectrosc.* **102**(2), 320-443 (1983).  
<sup>13</sup>M. K. Gilles, M. L. Polak and W. C. Lineberger, *J. Chem. Phys.* **95**(6), 4723-4 (1991).  
<sup>14</sup>A. Carrington, P. N. Dyer, and D. H. Levy, *J. Chem. Phys.* **52**(1), 309-14 (1970).  
<sup>15</sup>S. Saito, *J. Mol. Spectrosc.* **48**(3), 530-5 (1973).  
<sup>16</sup>J. M. Brown, C. R. Byfleet, B. J. Howard, and D. K. Russell, *Mol. Phys.* **23**(3), 457-68 (1972).  
<sup>17</sup>J. A. Coxon and D. A. Ramsay, *Can. J. Phys.* **54**, 1034 (1976).  
<sup>18</sup>A. Loewenschuss, J. C. Miller, and L. Andrews, *J. Mol. Spectrosc.* **80**(2), 351-62 (1980).  
<sup>19</sup>W. M. Vaidya, *Proc. Indian Acad. Sci.* **6A**, 122-8 (1937).  
<sup>20</sup>R. A. Durie, F. Legay, and D. A. Ramsay, *Can. J. Phys.* **38**, 444-52 (1960).  
<sup>21</sup>A. B. Callear and M. P. Metcalf, *Chem. Phys.* **20**(2), 233-42 (1977).

## Continued from page 1456

- <sup>3</sup>K. Bartsch and E. Wolf, *Z. anorg. allg. Chem.* **383**, 66 (1971).  
<sup>4</sup>H. C. Andersen and L. H. Belz, *J. Amer. Chem. Soc.* **75**, 4828 (1953).

## Continuation of discussions of selected I species

- <sup>5</sup>K. Uchimura, T. Takuma, M. Yuizumi, and T. Kunugi, *Kenki Kagaku* **35**, 876 (1967).  
<sup>6</sup>H. Schafer and B. Morcher, *Z. anorg. allg. Chem.* **352**, 122 (1967).  
<sup>7</sup>E. Wolf and C. Herbst, *Z. Chem.* **7**, 34 (1967).  
<sup>8</sup>R. J. H. Clark and D. M. Rippon, *J. Mol. Spectrosc.* **44**, 479 (1972).  
<sup>9</sup>M. W. Liston and L. E. Sutton, *Trans. Faraday Soc.* **37**, 393 (1941).  
<sup>10</sup>T. Shimanouchi, *NSRDS-NBS* **39**, (1972).  
<sup>11</sup>M. L. Delwaille, *J. Phys. Chem.* **56**, 355 (1952).  
<sup>12</sup>M. L. Delwaille and F. Francois, *J. Phys. Radium* **15**, 206 (1954).  
**Continued from page 1462**  
**References**  
<sup>1</sup>F. R. Sale and R. A. J. Shelton, *J. Less Common Metals* **3**, 54 (1965).  
<sup>2</sup>O. Rahlfs and W. Fischer, *Z. Anorg. Allg. Chem.* **211**, 349 (1933).  
<sup>3</sup>J. Gerlach, J. P. Krumme, F. Pawlek, and H. Probst, *Z. Phys. Chem. (Frankfurt am Main)* **53**, 135 (1967).  
<sup>4</sup>A. K. Baev and R. A. J. Shelton, *Russ. J. Phys. Chem.* **47**, 1340 (1973).  
<sup>5</sup>L. A. Niselson and T. D. Sokolova, *Russ. J. Inorg. Chem.* **7**, 1382 (1962).  
<sup>6</sup>R. J. H. Clark, B. K. Hunter and D. M. Rippon, *Chem. Ind. (London)* **1971**, 787 (1971), *Inorg. Chem.* **11**, 56 (1972).  
<sup>7</sup>R. J. H. Clark and D. M. Rippon, *J. Mol. Spectrosc.* **44**, 479 (1972); *Advan. Raman Spectrosc.* **1**, 443 (1972).  
<sup>8</sup>T. Shimanouchi, *J. Phys. Chem. Ref. Data* **3**, 269 (1971).  
<sup>9</sup>E. Z. Zasoren, G. V. Girichev, V. P. Spiridonov, K. S. Karsnov, and V. I. Tsirel'nikov, *Izv. Vysst. Ucheb. Zaved., Khim. Khim. Teknol.* **16**, 802 (1973).